

9H-xanthen-9-ol

Inchi:	InChI=1S/C13H10O2/c14-13-9-5-1-3-7-11(9)15-12-8-4-2-6-10(12)13/h1-8,13-14H
InchiKey:	JFRMYMMIJXLMBB-UHFFFAOYSA-N
Formula:	C13H10O2
SMILES:	OC1c2ccccc2Oc2ccccc21
Mol. weight [g/mol]:	198.22

Physical Properties

Property code	Value	Unit	Source
gf	114.05	kJ/mol	Joback Method
hf	-66.80	kJ/mol	Joback Method
hfus	29.03	kJ/mol	Joback Method
hvap	71.34	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.874		Crippen Method
mcvol	147.390	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	681.76	K	Joback Method
tc	912.27	K	Joback Method
tf	423.00	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.69	J/molxK	720.18	Joback Method
cpg	409.50	J/molxK	758.60	Joback Method
cpg	419.52	J/molxK	797.02	Joback Method
cpg	428.83	J/molxK	835.43	Joback Method
cpg	437.54	J/molxK	873.85	Joback Method
cpg	445.74	J/molxK	912.27	Joback Method
cpg	386.99	J/molxK	681.76	Joback Method
dvisc	0.0010997	Paxs	466.13	Joback Method
dvisc	0.0006714	Paxs	509.25	Joback Method
dvisc	0.0004427	Paxs	552.38	Joback Method

dvisc	0.0003101	Paxs	595.51	Joback Method
dvisc	0.0002279	Paxs	638.63	Joback Method
dvisc	0.0001741	Paxs	681.76	Joback Method
dvisc	0.0019920	Paxs	423.00	Joback Method
psub	3.74e-04	kPa	349.17	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.26e-04	kPa	343.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.32e-04	kPa	343.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.16e-04	kPa	343.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.62e-04	kPa	345.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.75e-04	kPa	345.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.60e-04	kPa	345.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)

psub	3.36e-04	kPa	347.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	3.32e-04	kPa	347.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	3.10e-04	kPa	347.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	4.36e-04	kPa	349.17	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.64e-04	kPa	341.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	3.88e-04	kPa	349.17	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	5.41e-04	kPa	351.07	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)

psub	5.56e-04	kPa	351.07	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	5.35e-04	kPa	351.07	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	6.85e-04	kPa	353.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	6.41e-04	kPa	353.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	6.13e-04	kPa	353.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	8.79e-04	kPa	355.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	7.53e-04	kPa	355.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)

psub	7.63e-04	kPa	355.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.81e-04	kPa	341.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.84e-04	kPa	341.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.32e-04	kPa	339.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.35e-04	kPa	339.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.52e-04	kPa	339.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.04e-04	kPa	337.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)

psub	1.13e-04	kPa	337.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	1.05e-04	kPa	337.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	7.79e-05	kPa	335.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	8.17e-05	kPa	335.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	8.54e-05	kPa	335.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	6.28e-05	kPa	333.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)
psub	5.67e-05	kPa	333.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH ₂)

psub

6.91e-05

kPa

333.18

Experimental and
computational
thermochemical
studies of
9-R-xanthene
derivatives
(R=OH, COOH,
CONH₂)

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH₂):	https://www.doi.org/10.1016/j.jct.2012.03.017

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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