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/mol×K	720.18	Joback Method
cpg	409.50	J/mol×K	758.60	Joback Method
cpg	419.52	J/mol×K	797.02	Joback Method
cpg	428.83	J/mol×K	835.43	Joback Method
cpg	437.54	J/mol×K	873.85	Joback Method
cpg	445.74	J/mol×K	912.27	Joback Method
cpg	386.99	J/mol×K	681.76	Joback Method
dvisc	0.0010997	Pa×s	466.13	Joback Method
dvisc	0.0006714	Pa×s	509.25	Joback Method
dvisc	0.0004427	Pa×s	552.38	Joback Method

dvisc	0.0003101	Pa×s	595.51	Joback Method
dvisc	0.0002279	Pa×s	638.63	Joback Method
dvisc	0.0001741	Pa×s	681.76	Joback Method
dvisc	0.0019920	Pa×s	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, CONH2)	
psub	5.35e-04	kPa	351.07	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	6.85e-04	kPa	353.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	6.41e-04	kPa	353.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	6.13e-04	kPa	353.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	8.79e-04	kPa	355.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	7.53e-04	kPa	355.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	

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, CONH2)	
psub	1.05e-04	kPa	337.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	7.79e-05	kPa	335.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	8.17e-05	kPa	335.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	8.54e-05	kPa	335.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	6.28e-05	kPa	333.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	5.67e-05	kPa	333.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	

psub	6.91e-05	kPa	333.18	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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