

9H-xanthene-9-carboxylic acid

Other names:	9-xanthenecarboxylic acid
Inchi:	InChI=1S/C14H10O3/c15-14(16)13-9-5-1-3-7-11(9)17-12-8-4-2-6-10(12)13/h1-8,13H,(H,
InchiKey:	VSBFNCXKYIEYIS-UHFFFAOYSA-N
Formula:	C14H10O3
SMILES:	O=C(O)C1c2ccccc2Oc2ccccc21
Mol. weight [g/mol]:	226.23

Physical Properties

Property code	Value	Unit	Source
gf	-6.45	kJ/mol	Joback Method
hf	-200.02	kJ/mol	Joback Method
hfus	33.22	kJ/mol	Joback Method
hvap	80.31	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	3.009		Crippen Method
mcvol	163.050	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
tb	758.51	K	Joback Method
tc	990.34	K	Joback Method
tf	484.20	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.77	J/molxK	990.34	Joback Method
cpg	458.17	J/molxK	797.15	Joback Method
cpg	468.10	J/molxK	835.79	Joback Method
cpg	477.32	J/molxK	874.42	Joback Method
cpg	485.94	J/molxK	913.06	Joback Method
cpg	494.06	J/molxK	951.70	Joback Method
cpg	447.46	J/molxK	758.51	Joback Method
dvisc	0.0001898	Paxs	712.79	Joback Method
dvisc	0.0002547	Paxs	667.07	Joback Method

dvisc	0.0003568	Paxs	621.36	Joback Method	
dvisc	0.0005273	Paxs	575.64	Joback Method	
dvisc	0.0008337	Paxs	529.92	Joback Method	
dvisc	0.0001466	Paxs	758.51	Joback Method	
dvisc	0.0014372	Paxs	484.20	Joback Method	
hvapt	125.50	kJ/mol	298.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	1.73e-04	kPa	387.25	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	1.62e-04	kPa	387.25	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	2.17e-04	kPa	389.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	2.12e-04	kPa	389.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	2.05e-04	kPa	389.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	2.58e-04	kPa	391.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	

psub	2.45e-04	kPa	391.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	3.15e-04	kPa	393.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.35e-04	kPa	385.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	3.81e-04	kPa	395.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	3.78e-04	kPa	395.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	3.65e-04	kPa	395.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	4.81e-04	kPa	397.11	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)

psub	4.63e-04	kPa	397.11	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	5.60e-04	kPa	399.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	5.45e-04	kPa	399.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	5.52e-04	kPa	399.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	6.83e-04	kPa	401.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	6.94e-04	kPa	401.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	6.74e-04	kPa	401.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)

psub	8.36e-04	kPa	403.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	8.29e-04	kPa	403.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	7.82e-04	kPa	403.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	9.64e-04	kPa	405.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	9.41e-04	kPa	405.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.43e-04	kPa	385.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.48e-04	kPa	385.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)

psub	1.13e-04	kPa	383.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.12e-04	kPa	383.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.19e-04	kPa	383.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.69e-04	kPa	387.25	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	3.06e-04	kPa	393.14	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/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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

<https://www.doi.org/10.1016/j.jct.2012.03.017>

https://en.wikipedia.org/wiki/Joback_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
hvapt:	Enthalpy of vaporization at a given temperature
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

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