

2-hydroxy-1,8-cineole I

Inchi:	InChI=1S/C10H18O2/c1-9(2)7-4-5-10(3,12-9)8(11)6-7/h7-8,11H,4-6H2,1-3H3/t7?,8?,10-
InchiKey:	YVCUGZBVCHODNB-KTOWXAHTSA-N
Formula:	C10H18O2
SMILES:	CC1(C)OC2(C)CCC1CC2O
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-118.72	kJ/mol	Joback Method
hf	-410.88	kJ/mol	Joback Method
hfus	15.34	kJ/mol	Joback Method
hvap	56.29	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.715		Crippen Method
mcvol	141.780	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinsol	1239.00		NIST Webbook
tb	560.49	K	Joback Method
tc	767.10	K	Joback Method
tf	358.01	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.49	J/mol×K	560.49	Joback Method
cpg	402.41	J/mol×K	594.92	Joback Method
cpg	417.30	J/mol×K	629.36	Joback Method
cpg	431.35	J/mol×K	663.79	Joback Method
cpg	444.77	J/mol×K	698.23	Joback Method
cpg	457.73	J/mol×K	732.66	Joback Method
cpg	470.44	J/mol×K	767.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R415913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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