4-hydroxy-1,8-cineole

Inchi: InChI=1S/C10H18O2/c1-8(2)10(11)6-4-9(3,12-8)5-7-10/h11H,4-7H2,1-3H3/t9-,10?
InchiKey: UOAXJWKFKLGEOQ-OKXAEBFBSA-N
Formula: C10H18O2
SMILES: CC12CCC(O)(CC1)C(C)(C)O2
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-116.50	kJ/mol	Joback Method
hf	-375.30	kJ/mol	Joback Method
hfus	7.97	kJ/mol	Joback Method
hvap	55.45	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.859		Crippen Method
mcvol	141.780	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1187.00		NIST Webbook
ripol	1993.00		NIST Webbook
tb	565.40	K	Joback Method
tc	780.32	K	Joback Method
tf	386.15	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.91	J/mol×K	565.40	Joback Method
cpg	399.05	J/mol×K	601.22	Joback Method
cpg	413.11	J/mol×K	637.04	Joback Method
cpg	426.41	J/mol×K	672.86	Joback Method
cpg	439.25	J/mol×K	708.68	Joback Method
cpg	451.93	J/mol×K	744.50	Joback Method
cpg	464.77	J/mol×K	780.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R404210&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume