

9-hydroxy-1,8-cineole

Inchi:	InChI=1S/C10H18O2/c1-9-5-3-8(4-6-9)10(2,7-11)12-9/h8,11H,3-7H2,1-2H3/t8?,9-,10-/m
InchiKey:	HTGSXANWVMWFEM-AGROOBSYSA-N
Formula:	C10H18O2
SMILES:	CC12CCC(CC1)C(C)(CO)O2
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-111.01	kJ/mol	Joback Method
hf	-390.54	kJ/mol	Joback Method
hfus	14.27	kJ/mol	Joback Method
hvap	56.60	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.717		Crippen Method
mcvol	141.780	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	1340.00		NIST Webbook
rinpol	1267.00		NIST Webbook
ripol	2091.00		NIST Webbook
tb	565.16	K	Joback Method
tc	771.88	K	Joback Method
tf	362.25	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.13	J/molxK	565.16	Joback Method
cpg	400.59	J/molxK	599.61	Joback Method
cpg	415.03	J/molxK	634.07	Joback Method
cpg	428.66	J/molxK	668.52	Joback Method
cpg	441.67	J/molxK	702.98	Joback Method
cpg	454.27	J/molxK	737.43	Joback Method
cpg	466.66	J/molxK	771.88	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R404230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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