m-Cineol

Inchi: InChI=1S/C10H18O/c1-8(2)10-6-4-5-9(3,7-10)11-10/h8H,4-7H2,1-3H3
InchiKey: ZQNCDTINDGYLTB-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC(C)C12CCCC(C)(C1)O2
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	43.18	kJ/mol	Joback Method
hf	-217.09	kJ/mol	Joback Method
hfus	7.69	kJ/mol	Joback Method
hvap	39.67	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.744		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	1040.00		NIST Webbook
rinpol	1040.00		NIST Webbook
tb	472.94	K	Joback Method
tc	692.30	K	Joback Method
tf	294.19	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.61	J/mol×K	472.94	Joback Method
cpg	340.77	J/mol×K	509.50	Joback Method
cpg	358.18	J/mol×K	546.06	Joback Method
cpg	374.12	J/mol×K	582.62	Joback Method
cpg	388.82	J/mol×K	619.18	Joback Method
cpg	402.55	J/mol×K	655.74	Joback Method
cpg	415.56	J/mol×K	692.30	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R325003&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume