2-Oxabicyclo[2.2.2]octan-6-one, 1,3,3-trimethyl-

Other names: 2-Oxocineole
Inchi: InChI=1S/C10H16O2/c1-9(2)7-4-5-10(3,12-9)8(11)6-7/h7H,4-6H2,1-3H3
InchiKey: CCBAAZXPXFYPBE-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC12CCC(CC1=O)C(C)(C)O2
Mol. weight [g/mol]: 168.23
CAS: 107598-08-3

Physical Properties

Property code	Value	Unit	Source
gf	-96.78	kJ/mol	Joback Method
hf	-376.01	kJ/mol	Joback Method
hfus	9.69	kJ/mol	Joback Method
hvap	44.17	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.923		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1217.00		NIST Webbook
rinpol	1217.00		NIST Webbook
tb	540.80	K	Joback Method
tc	780.01	K	Joback Method
tf	369.65	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.06	J/mol×K	540.80	Joback Method
cpg	374.39	J/mol×K	580.67	Joback Method
cpg	391.40	J/mol×K	620.54	Joback Method
cpg	407.37	J/mol×K	660.41	Joback Method
cpg	422.55	J/mol×K	700.27	Joback Method
cpg	437.20	J/mol×K	740.14	Joback Method

cpg	451.60	J/mol×K	780.01	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=C107598083&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