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]: 168.24

Physical Properties

Property code	Value	Unit	Source
hf	-386.84	kJ/mol	Cheméo Relay (1.0)
hfus	9.69	kJ/mol	Joback Method
hvap	52.14	kJ/mol	Cheméo Relay (1.0)
ie	8.76	eV	Cheméo Relay (1.0)
log10ws	-1.26		Cheméo Relay (1.0)
logp	1.923		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
rinpol	1217.00		NIST Webbook
rinpol	1217.00		NIST Webbook
tb	478.24	K	Cheméo Relay (1.0)
tf	398.03	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107598083&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point