exo-2-Hydroxycineole acetate

Other names:	1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octan-6-ol, acetate
	2-acetoxy-1,8-cineole
	exo-2-hydroxycineol acetate
	1,3,3-trimethyl-2-oxabicyclo[2.2.2]octan-6-yl acetate
	2-Hydroxycineole, acetate
Inchi:	InChI=1S/C12H20O3/c1-8(13)14-10-7-9-5-6-12(10,4)15-11(9,2)3/h9-10H,5-7H2,1-4H3
InchiKey:	XRKZFZWIYZDOQO-UHFFFAOYSA-N
Formula:	C12H20O3
SMILES:	CC(=O)OC1CC2CCC1(C)OC2(C)C
Mol. weight [g/mol]:	212.29
CAS:	72257-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-198.98	kJ/mol	Joback Method
hf	-544.73	kJ/mol	Joback Method
hfus	19.22	kJ/mol	Joback Method
hvap	53.22	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.286		Crippen Method
mcvol	171.530	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1352.00		NIST Webbook
rinpol	1367.60		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1339.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	590.36	K	Joback Method
tc	811.40	K	Joback Method
tf	391.89	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.00	J/mol×K	590.36	Joback Method
cpg	490.68	J/mol×K	627.20	Joback Method
cpg	508.27	J/mol×K	664.04	Joback Method
cpg	525.00	J/mol×K	700.88	Joback Method
cpg	541.09	J/mol×K	737.72	Joback Method
cpg	556.75	J/mol×K	774.56	Joback Method
cpg	572.21	J/mol×K	811.40	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=C72257535&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume