cis-1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octan-5-ol

Inchi: InChI=1S/C10H18O2/c1-9(2)7-4-5-10(3,12-9)6-8(7)11/h7-8,11H,4-6H2,1-3H3
InchiKey: WHIKIYRWRMRQNK-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC12CCC(C(O)C1)C(C)(C)O2
Mol. weight [g/mol]: 170.25
CAS: 98920-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-118.72	kJ/mol	Joback Method
hf	-410.88	kJ/mol	Joback Method
hfus	15.34	kJ/mol	Joback Method
hvap	56.29	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.715		Crippen Method
mcvol	141.780	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
ripol	1864.00		NIST Webbook
tb	560.49	K	Joback Method
tc	767.10	K	Joback Method
tf	358.01	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.49	J/mol×K	560.49	Joback Method
cpg	402.41	J/mol×K	594.92	Joback Method
cpg	417.30	J/mol×K	629.36	Joback Method
cpg	431.35	J/mol×K	663.79	Joback Method
cpg	444.77	J/mol×K	698.23	Joback Method
cpg	457.73	J/mol×K	732.66	Joback Method

cpg	470.44	J/mol×K	767.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98920242&Units=SI
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

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