3,3-Dimethyl-5-0xa bicyclo[2.4.0]octan-2-ol

Inchi: InChI=1S/C9H16O2/c1-9(2)7(10)6-4-3-5-11-8(6)9/h6-8,10H,3-5H2,1-2H3
InchiKey: OGUSPLVPTTWVRC-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CC1(C)C(O)C2CCCOC21
Mol. weight [g/mol]: 156.22
CAS: 90646-73-4

Physical Properties

Property code	Value	Unit	Source
gf	-121.65	kJ/mol	Joback Method
hf	-405.48	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	55.22	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.182		Crippen Method
mcvol	127.690	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	537.37	K	Joback Method
tc	739.11	K	Joback Method
tf	322.84	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.52	J/mol×K	537.37	Joback Method
cpg	355.12	J/mol×K	570.99	Joback Method
cpg	369.74	J/mol×K	604.62	Joback Method
cpg	383.49	J/mol×K	638.24	Joback Method
cpg	396.48	J/mol×K	671.87	Joback Method
cpg	408.81	J/mol×K	705.49	Joback Method
cpg	420.59	J/mol×K	739.11	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=C90646734&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume