1,3-Cyclobutanediol, 2,2,4,4-tetramethyl-, monoformate

Inchi: InChI=1S/C9H16O3/c1-8(2)6(11)9(3,4)7(8)12-5-10/h5-7,11H,1-4H3
InchiKey: ZTLMFFPGDIVCRP-UHFFFAOYSA-N
Formula: C9H16O3
SMILES: CC1(C)C(O)C(C)(C)C1OC=O
Mol. weight [g/mol]: 172.22
CAS: 116373-50-3

Physical Properties

Property code	Value	Unit	Source
gf	-301.90	kJ/mol	Joback Method
hf	-563.02	kJ/mol	Joback Method
hfus	13.28	kJ/mol	Joback Method
hvap	58.29	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	0.955		Crippen Method
mcvol	140.120	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	566.06	K	Joback Method
tc	757.93	K	Joback Method
tf	365.74	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.29	J/mol×K	566.06	Joback Method
cpg	382.11	J/mol×K	598.04	Joback Method
cpg	394.27	J/mol×K	630.02	Joback Method
cpg	405.89	J/mol×K	662.00	Joback Method
cpg	417.10	J/mol×K	693.98	Joback Method
cpg	428.03	J/mol×K	725.96	Joback Method
cpg	438.79	J/mol×K	757.93	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=C116373503&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume