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

Inchi: InChI=1S/C14H26O3/c1-6-7-8-9-10(15)17-12-13(2,3)11(16)14(12,4)5/h11-12,16H,6-9H2

InchiKey: SEXQLQZUVYMARV-UHFFFAOYSA-N

Formula: C14H26O3

SMILES: CCCCCC(=O)OC1C(C)(C)C(O)C1(C)C

Mol. weight [g/mol]: 242.35

CAS: 116373-51-4

Physical Properties

Property code	Value	Unit	Source
gf	-289.20	kJ/mol	Joback Method
hf	-693.22	kJ/mol	Joback Method
hfus	25.54	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.905		Crippen Method
mcvol	210.570	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
tb	685.67	K	Joback Method
tc	872.04	K	Joback Method
tf	430.02	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.19	J/mol×K	685.67	Joback Method
cpg	640.62	J/mol×K	716.73	Joback Method
cpg	656.57	J/mol×K	747.79	Joback Method
cpg	672.17	J/mol×K	778.85	Joback Method
cpg	687.55	J/mol×K	809.91	Joback Method
cpg	702.82	J/mol×K	840.98	Joback Method
cpg	718.11	J/mol×K	872.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373514&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

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