1,3-Cyclobutanediol, 2,2,4,4-tetramethyl-, mono(2-ethylhexanoate)

Inchi: InChI=1S/C16H30O3/c1-7-9-10-11(8-2)12(17)19-14-15(3,4)13(18)16(14,5)6/h11,13-14,1
InchiKey: TVOOJZKUWKRRCV-UHFFFAOYSA-N
Formula: C16H30O3
SMILES: CCCCC(CC)C(=O)OC1C(C)(C)C(O)C1(C)C
Mol. weight [g/mol]: 270.41
CAS: 116373-48-9

Physical Properties

Property code	Value	Unit	Source
gf	-274.80	kJ/mol	Joback Method
hf	-739.78	kJ/mol	Joback Method
hfus	27.20	kJ/mol	Joback Method
hvap	73.51	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.542		Crippen Method
mcvol	238.750	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
tb	730.99	K	Joback Method
tc	918.31	K	Joback Method
tf	437.56	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.96	J/mol×K	730.99	Joback Method
cpg	754.93	J/mol×K	762.21	Joback Method
cpg	772.49	J/mol×K	793.43	Joback Method
cpg	789.77	J/mol×K	824.65	Joback Method
cpg	806.89	J/mol×K	855.87	Joback Method
cpg	824.00	J/mol×K	887.09	Joback Method
cpg	841.20	J/mol×K	918.31	Joback Method

Sources

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=C116373489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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