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

Other names: 1,3-Cyclobutanediol, 2,2,4,4-tetramethyl-, monononanoate
Inchi: InChI=1S/C17H32O3/c1-6-7-8-9-10-11-12-13(18)20-15-16(2,3)14(19)17(15,4)5/h14-15,1
InchiKey: YRNWBGBHAJATKE-UHFFFAOYSA-N
Formula: C17H32O3
SMILES: CCCCCCCCC(=O)OC1C(C)(C)C(O)C1(C)C
Mol. weight [g/mol]: 284.43
CAS: 116373-52-5

Physical Properties

Property code	Value	Unit	Source
gf	-263.94	kJ/mol	Joback Method
hf	-755.14	kJ/mol	Joback Method
hfus	33.31	kJ/mol	Joback Method
hvap	76.13	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.076		Crippen Method
mcvol	252.840	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
tb	754.31	K	Joback Method
tc	939.50	K	Joback Method
tf	463.83	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.58	J/mol×K	754.31	Joback Method
cpg	813.03	J/mol×K	785.18	Joback Method
cpg	831.13	J/mol×K	816.04	Joback Method
cpg	849.01	J/mol×K	846.91	Joback Method
cpg	866.79	J/mol×K	877.77	Joback Method
cpg	884.60	J/mol×K	908.64	Joback Method
cpg	902.56	J/mol×K	939.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373525&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