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

Inchi: InChI=1S/C10H18O3/c1-6(11)13-8-9(2,3)7(12)10(8,4)5/h7-8,12H,1-5H3
InchiKey: VPAHAVKFSSDLPN-UHFFFAOYSA-N
Formula: C10H18O3
SMILES: CC(=O)OC1C(C)(C)C(O)C1(C)C
Mol. weight [g/mol]: 186.25
CAS: 116373-49-0

Physical Properties

Property code	Value	Unit	Source
gf	-322.88	kJ/mol	Joback Method
hf	-610.66	kJ/mol	Joback Method
hfus	15.18	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.345		Crippen Method
mcvol	154.210	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
tb	594.15	K	Joback Method
tc	787.83	K	Joback Method
tf	384.94	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.57	J/mol×K	594.15	Joback Method
cpg	430.40	J/mol×K	626.43	Joback Method
cpg	443.60	J/mol×K	658.71	Joback Method
cpg	456.30	J/mol×K	690.99	Joback Method
cpg	468.63	J/mol×K	723.27	Joback Method
cpg	480.71	J/mol×K	755.55	Joback Method
cpg	492.68	J/mol×K	787.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373490&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