1,3-Propanediol, 2-hydroxymethyl-2-methyl-, triacetate

Inchi: InChI=1S/C11H18O6/c1-8(12)15-5-11(4,6-16-9(2)13)7-17-10(3)14/h5-7H2,1-4H3
InchiKey: PXZWZRWNBAERBU-UHFFFAOYSA-N
Formula: C11H18O6
SMILES: CC(=O)OCC(C)(COC(C)=O)COC(C)=O
Mol. weight [g/mol]: 246.26
CAS: 13431-59-9

Physical Properties

Property code	Value	Unit	Source
gf	-657.18	kJ/mol	Joback Method
hf	-1013.52	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	66.25	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.682		Crippen Method
mcvol	188.170	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
tb	676.72	K	Joback Method
tc	870.40	K	Joback Method
tf	432.63	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.17	J/mol×K	676.72	Joback Method
cpg	526.28	J/mol×K	709.00	Joback Method
cpg	538.64	J/mol×K	741.28	Joback Method
cpg	550.26	J/mol×K	773.56	Joback Method
cpg	561.14	J/mol×K	805.84	Joback Method
cpg	571.27	J/mol×K	838.12	Joback Method
cpg	580.66	J/mol×K	870.40	Joback Method
dvisc	0.0010614	Pa×s	432.63	Joback Method
dvisc	0.0006218	Pa×s	473.31	Joback Method

dvisc	0.0003964	Pa×s	513.99	Joback Method
dvisc	0.0002700	Pa×s	554.68	Joback Method
dvisc	0.0001938	Pa×s	595.36	Joback Method
dvisc	0.0001451	Pa×s	636.04	Joback Method
dvisc	0.0001125	Pa×s	676.72	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13431599&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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