1,3,5-tris-(Hydroxymethyl)cyclohexane, triacetate

Inchi: InChI=1S/C15H24O6/c1-10(16)19-7-13-4-14(8-20-11(2)17)6-15(5-13)9-21-12(3)18/h13-1

InchiKey: BSUAWZLOSIPEAI-UHFFFAOYSA-N

Formula: C15H24O6

SMILES: CC(=O)OCC1CC(COC(C)=O)CC(COC(C)=O)C1

Mol. weight [g/mol]: 300.35

Physical Properties

Property code	Value	Unit	Source
gf	-617.31	kJ/mol	Joback Method
hf	-1073.69	kJ/mol	Joback Method
hfus	36.94	kJ/mol	Joback Method
hvap	76.26	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.708		Crippen Method
mcvol	233.670	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	1998.00		NIST Webbook
tb	781.68	K	Joback Method
tc	985.04	K	Joback Method
tf	474.19	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.14	J/mol×K	781.68	Joback Method
cpg	745.83	J/mol×K	815.57	Joback Method
cpg	761.25	J/mol×K	849.47	Joback Method
cpg	775.40	J/mol×K	883.36	Joback Method
cpg	788.27	J/mol×K	917.25	Joback Method
cpg	799.82	J/mol×K	951.15	Joback Method
cpg	810.05	J/mol×K	985.04	Joback Method
dvisc	0.0009883	Pa×s	474.19	Joback Method
dvisc	0.0005963	Pa×s	525.44	Joback Method

dvisc	0.0003936	Pa×s	576.69	Joback Method
dvisc	0.0002780	Pa×s	627.93	Joback Method
dvisc	0.0002069	Pa×s	679.18	Joback Method
dvisc	0.0001606	Pa×s	730.43	Joback Method
dvisc	0.0001288	Pa×s	781.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R96365&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume