1,2,3 propanetriol diacetate

Other names: glycerol 1,3-di(acetate)
Inchi: InChI=1S/C7H12O5/c1-5(9)11-4-7(3-8)12-6(2)10/h7-8H,3-4H2,1-2H3
InchiKey: UXDDRFCJKNROTO-UHFFFAOYSA-N
Formula: C7H12O5
SMILES: CC(=O)OCC(CO)OC(C)=O
Mol. weight [g/mol]: 176.17
CAS: 25395-31-7

Physical Properties

Property code	Value	Unit	Source
chl	-3348.90 ± 6.70	kJ/mol	NIST Webbook
gf	-599.04	kJ/mol	Joback Method
hf	-834.92	kJ/mol	Joback Method
hfl	-1120.70 ± 6.70	kJ/mol	NIST Webbook
hfus	20.03	kJ/mol	Joback Method
hvap	65.78	kJ/mol	Joback Method
log10ws	0.15		Crippen Method
logp	-0.527		Crippen Method
mcvol	130.240	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
ripol	2299.00		NIST Webbook
ripol	2244.00		NIST Webbook
ripol	2299.00		NIST Webbook
ripol	2244.00		NIST Webbook
tb	603.88	K	Joback Method
tc	784.28	K	Joback Method
tf	358.79	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	325.66	J/mol×K	603.88	Joback Method
cpg	335.00	J/mol×K	633.95	Joback Method
cpg	343.95	J/mol×K	664.01	Joback Method
cpg	352.49	J/mol×K	694.08	Joback Method
cpg	360.63	J/mol×K	724.15	Joback Method
cpg	368.34	J/mol×K	754.22	Joback Method
cpg	375.62	J/mol×K	784.28	Joback Method
dvisc	0.0038673	Pa×s	358.79	Joback Method
dvisc	0.0014417	Pa×s	399.64	Joback Method
dvisc	0.0006454	Pa×s	440.49	Joback Method
dvisc	0.0003312	Pa×s	481.34	Joback Method
dvisc	0.0001886	Pa×s	522.18	Joback Method
dvisc	0.0001166	Pa×s	563.03	Joback Method
dvisc	0.0000769	Pa×s	603.88	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25395317&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume