Hexapropylene glycol, diacetate

Inchi: InChI=1S/C22H42O9/c1-15(9-26-17(3)11-28-19(5)13-30-21(7)23)25-10-16(2)27-12-18(4
InchiKey: XRODWTVLWCGTKT-UHFFFAOYSA-N
Formula: C22H42O9
SMILES: CC(=O)OCC(C)OCC(C)OCC(C)OCC(C)OCC(C)OCC(C)OC(C)=O
Mol. weight [g/mol]: 450.56

Physical Properties

Property code	Value	Unit	Source
gf	-873.12	kJ/mol	Joback Method
hf	-1679.79	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	92.60	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.527		Crippen Method
mcvol	365.070	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	2391.00		NIST Webbook
rinpol	2396.00		NIST Webbook
rinpol	2395.00		NIST Webbook
rinpol	2404.00		NIST Webbook
rinpol	2397.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2399.00		NIST Webbook
rinpol	2397.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
tb	964.80	K	Joback Method
tc	1183.03	K	Joback Method
tf	503.17	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1249.52	J/mol×K	964.80	Joback Method
cpg	1265.58	J/mol×K	1001.17	Joback Method
cpg	1279.41	J/mol×K	1037.54	Joback Method
cpg	1290.98	J/mol×K	1073.92	Joback Method
cpg	1300.23	J/mol×K	1110.29	Joback Method
cpg	1307.13	J/mol×K	1146.66	Joback Method
cpg	1311.62	J/mol×K	1183.03	Joback Method
dvisc	0.0002127	Pa×s	503.17	Joback Method
dvisc	0.0000750	Pa×s	580.11	Joback Method
dvisc	0.0000337	Pa×s	657.05	Joback Method
dvisc	0.0000180	Pa×s	733.99	Joback Method
dvisc	0.0000108	Pa×s	810.92	Joback Method
dvisc	0.0000071	Pa×s	887.86	Joback Method
dvisc	0.0000049	Pa×s	964.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R152137&Units=SI

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

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