Glycerol, 2,3-dimethyl, 1-heptadecanoate

Inchi: InChI=1S/C22H44O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22(23)26-20-21(25-3)1
InchiKey: LAVHQUSMQCEMCR-UHFFFAOYSA-N
Formula: C22H44O4
SMILES: CCCCCCCCCCCCCCCCC(=O)OCC(COC)OC
Mol. weight [g/mol]: 372.58

Physical Properties

Property code	Value	Unit	Source
gf	-312.00	kJ/mol	Joback Method
hf	-1011.93	kJ/mol	Joback Method
hfus	54.38	kJ/mol	Joback Method
hvap	78.15	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	6.062		Crippen Method
mcvol	340.020	ml/mol	McGowan Method
pc	912.73	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	823.45	K	Joback Method
tc	1008.38	K	Joback Method
tf	439.32	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.67	J/mol×K	823.45	Joback Method
cpg	1188.69	J/mol×K	977.56	Joback Method
cpg	1173.02	J/mol×K	946.74	Joback Method
cpg	1156.19	J/mol×K	915.91	Joback Method
cpg	1138.20	J/mol×K	885.09	Joback Method
cpg	1119.03	J/mol×K	854.27	Joback Method
cpg	1203.23	J/mol×K	1008.38	Joback Method
dvisc	0.0000287	Pa×s	823.45	Joback Method

dvisc	0.0000391	Pa×s	759.43	Joback Method
dvisc	0.0000565	Pa×s	695.41	Joback Method
dvisc	0.0000878	Pa×s	631.38	Joback Method
dvisc	0.0001510	Pa×s	567.36	Joback Method
dvisc	0.0002980	Pa×s	503.34	Joback Method
dvisc	0.0007170	Pa×s	439.32	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=R56478&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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