

Diglycolic acid, isoheptyl octyl ester

Inchi:	InChI=1S/C18H34O5/c1-4-5-6-7-8-9-12-22-17(19)14-21-15-18(20)23-13-10-11-16(2)3/h1
InchiKey:	LORPJZRBSIYJJP-UHFFFAOYSA-N
Formula:	C18H34O5
SMILES:	CCCCCCCCOC(=O)COCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	330.46

Physical Properties

Property code	Value	Unit	Source
gf	-474.60	kJ/mol	Joback Method
hf	-1041.95	kJ/mol	Joback Method
hfus	45.61	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.886		Crippen Method
mvol	285.230	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
tb	785.80	K	Joback Method
tc	967.95	K	Joback Method
tf	444.17	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.97	J/molxK	785.80	Joback Method
cpg	957.65	J/molxK	937.59	Joback Method
cpg	944.29	J/molxK	907.23	Joback Method
cpg	929.94	J/molxK	876.87	Joback Method
cpg	914.61	J/molxK	846.52	Joback Method
cpg	898.29	J/molxK	816.16	Joback Method
cpg	970.03	J/molxK	967.95	Joback Method
dvisc	0.0000489	Paxs	785.80	Joback Method

dvisc	0.0000653	Paxs	728.86	Joback Method
dvisc	0.0000915	Paxs	671.92	Joback Method
dvisc	0.0001365	Paxs	614.98	Joback Method
dvisc	0.0002209	Paxs	558.05	Joback Method
dvisc	0.0003989	Paxs	501.11	Joback Method
dvisc	0.0008380	Paxs	444.17	Joback Method

Sources

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=U382113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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