

Diglycolic acid, heptyl octyl ester

Inchi:	InChI=1S/C19H36O5/c1-3-5-7-9-11-13-15-24-19(21)17-22-16-18(20)23-14-12-10-8-6-4-2
InchiKey:	UQSJMHHKXZOIPG-UHFFFAOYSA-N
Formula:	C19H36O5
SMILES:	CCCCCCCCOC(=O)COCC(=O)OCCCCCCC
Mol. weight [g/mol]:	344.49

Physical Properties

Property code	Value	Unit	Source
gf	-463.74	kJ/mol	Joback Method
hf	-1057.31	kJ/mol	Joback Method
hfus	51.73	kJ/mol	Joback Method
hvap	78.61	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.420		Crippen Method
mvol	299.320	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	2878.00		NIST Webbook
rinpol	2878.00		NIST Webbook
tb	809.12	K	Joback Method
tc	992.99	K	Joback Method
tf	470.44	K	Joback Method
vc	1.165	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.26	J/molxK	809.12	Joback Method
cpg	1017.95	J/molxK	962.34	Joback Method
cpg	1004.48	J/molxK	931.70	Joback Method
cpg	989.99	J/molxK	901.05	Joback Method
cpg	974.45	J/molxK	870.41	Joback Method
cpg	957.88	J/molxK	839.76	Joback Method
cpg	1030.39	J/molxK	992.99	Joback Method
dvisc	0.0000461	Paxs	809.12	Joback Method

dvisc	0.0000606	Paxs	752.67	Joback Method
dvisc	0.0000834	Paxs	696.23	Joback Method
dvisc	0.0001213	Paxs	639.78	Joback Method
dvisc	0.0001897	Paxs	583.33	Joback Method
dvisc	0.0003267	Paxs	526.89	Joback Method
dvisc	0.0006407	Paxs	470.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382115&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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