

Diglycolic acid, isoheptyl 2-octyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-477.04	kJ/mol	Joback Method
hf	-1047.23	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	75.61	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.885		Crippen Method
mvol	285.230	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2587.00		NIST Webbook
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tb	785.36	K	Joback Method
tc	968.70	K	Joback Method
tf	429.17	K	Joback Method
vc	1.097	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.46	J/molxK	785.36	Joback Method
cpg	898.90	J/molxK	815.92	Joback Method
cpg	915.32	J/molxK	846.47	Joback Method
cpg	930.73	J/molxK	877.03	Joback Method
cpg	945.13	J/molxK	907.59	Joback Method
cpg	958.52	J/molxK	938.14	Joback Method
cpg	970.92	J/molxK	968.70	Joback Method
dvisc	0.0010058	Paxs	429.17	Joback Method

dvisc	0.0004376	Paxs	488.53	Joback Method
dvisc	0.0002280	Paxs	547.90	Joback Method
dvisc	0.0001349	Paxs	607.26	Joback Method
dvisc	0.0000877	Paxs	666.63	Joback Method
dvisc	0.0000611	Paxs	726.00	Joback Method
dvisc	0.0000450	Paxs	785.36	Joback Method

Sources

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=U382320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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