

Diglycolic acid, propyl undecyl ester

Inchi:	InChI=1S/C18H34O5/c1-3-5-6-7-8-9-10-11-12-14-23-18(20)16-21-15-17(19)22-13-4-2/h3
InchiKey:	FKVUVEXCVGYDSW-UHFFFAOYSA-N
Formula:	C18H34O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCCC
Mol. weight [g/mol]:	330.46

Physical Properties

Property code	Value	Unit	Source
gf	-472.16	kJ/mol	Joback Method
hf	-1036.67	kJ/mol	Joback Method
hfus	49.14	kJ/mol	Joback Method
hvap	76.38	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	4.030		Crippen Method
mvol	285.230	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	2781.00		NIST Webbook
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tb	786.24	K	Joback Method
tc	967.32	K	Joback Method
tf	459.17	K	Joback Method
vc	1.109	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.48	J/molxK	786.24	Joback Method
cpg	897.68	J/molxK	816.42	Joback Method
cpg	913.92	J/molxK	846.60	Joback Method
cpg	929.18	J/molxK	876.78	Joback Method
cpg	943.48	J/molxK	906.96	Joback Method
cpg	956.81	J/molxK	937.14	Joback Method
cpg	969.19	J/molxK	967.32	Joback Method
dvisc	0.0007129	Paxs	459.17	Joback Method

dvisc	0.0003677	Paxs	513.68	Joback Method
dvisc	0.0002154	Paxs	568.19	Joback Method
dvisc	0.0001386	Paxs	622.71	Joback Method
dvisc	0.0000957	Paxs	677.22	Joback Method
dvisc	0.0000698	Paxs	731.73	Joback Method
dvisc	0.0000532	Paxs	786.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381862&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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