

Diglycolic acid, heptyl neopentyl ester

Inchi:	InChI=1S/C16H30O5/c1-5-6-7-8-9-10-20-14(17)11-19-12-15(18)21-13-16(2,3)4/h5-13H2
InchiKey:	ULNLYJYVOYAJEU-UHFFFAOYSA-N
Formula:	C16H30O5
SMILES:	CCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	302.41

Physical Properties

Property code	Value	Unit	Source
gf	-486.16	kJ/mol	Joback Method
hf	-1004.14	kJ/mol	Joback Method
hfus	36.54	kJ/mol	Joback Method
hvap	70.64	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	3.106		Crippen Method
mvol	257.050	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	2381.00		NIST Webbook
rinpol	2381.00		NIST Webbook
tb	737.25	K	Joback Method
tc	919.61	K	Joback Method
tf	439.05	K	Joback Method
vc	0.987	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.53	J/molxK	737.25	Joback Method
cpg	782.11	J/molxK	767.64	Joback Method
cpg	797.78	J/molxK	798.04	Joback Method
cpg	812.56	J/molxK	828.43	Joback Method
cpg	826.46	J/molxK	858.82	Joback Method
cpg	839.49	J/molxK	889.21	Joback Method
cpg	851.66	J/molxK	919.61	Joback Method
dvisc	0.0008535	Paxs	439.05	Joback Method

dvisc	0.0004344	Paxs	488.75	Joback Method
dvisc	0.0002504	Paxs	538.45	Joback Method
dvisc	0.0001585	Paxs	588.15	Joback Method
dvisc	0.0001077	Paxs	637.85	Joback Method
dvisc	0.0000774	Paxs	687.55	Joback Method
dvisc	0.0000581	Paxs	737.25	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=U381920&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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