

Diglycolic acid, pentyl octyl ester

Inchi:	InChI=1S/C17H32O5/c1-3-5-7-8-9-11-13-22-17(19)15-20-14-16(18)21-12-10-6-4-2/h3-15
InchiKey:	IOHNECXTVHULPV-UHFFFAOYSA-N
Formula:	C17H32O5
SMILES:	CCCCCCCCOC(=O)COCC(=O)OCCCCC
Mol. weight [g/mol]:	316.43

Physical Properties

Property code	Value	Unit	Source
gf	-480.58	kJ/mol	Joback Method
hf	-1016.03	kJ/mol	Joback Method
hfus	46.55	kJ/mol	Joback Method
hvap	74.16	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.640		Crippen Method
mvol	271.140	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	763.36	K	Joback Method
tc	942.36	K	Joback Method
tf	447.90	K	Joback Method
vc	1.054	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.57	J/molxK	763.36	Joback Method
cpg	838.37	J/molxK	793.19	Joback Method
cpg	854.26	J/molxK	823.03	Joback Method
cpg	869.24	J/molxK	852.86	Joback Method
cpg	883.32	J/molxK	882.69	Joback Method
cpg	896.49	J/molxK	912.53	Joback Method
cpg	908.76	J/molxK	942.36	Joback Method
dvisc	0.0007897	Paxs	447.90	Joback Method

dvisc	0.0004124	Paxs	500.48	Joback Method
dvisc	0.0002437	Paxs	553.05	Joback Method
dvisc	0.0001578	Paxs	605.63	Joback Method
dvisc	0.0001095	Paxs	658.21	Joback Method
dvisc	0.0000802	Paxs	710.78	Joback Method
dvisc	0.0000613	Paxs	763.36	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=U382112&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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