

Diglycolic acid, pentyl 3-phenylpropyl ester

Inchi:	InChI=1S/C18H26O5/c1-2-3-7-12-22-17(19)14-21-15-18(20)23-13-8-11-16-9-5-4-6-10-16
InchiKey:	FRZBDHRIYPBUPL-UHFFFAOYSA-N
Formula:	C18H26O5
SMILES:	CCCCCOC(=O)COCC(=O)OCCCC1CCCCC1
Mol. weight [g/mol]:	322.40

Physical Properties

Property code	Value	Unit	Source
gf	-359.75	kJ/mol	Joback Method
hf	-800.14	kJ/mol	Joback Method
hfus	43.18	kJ/mol	Joback Method
hvap	78.66	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.912		Crippen Method
mvol	261.470	ml/mol	McGowan Method
pc	1550.00	kPa	Joback Method
rmpol	3011.00		NIST Webbook
rmpol	3011.00		NIST Webbook
tb	812.92	K	Joback Method
tc	1012.09	K	Joback Method
tf	485.59	K	Joback Method
vc	1.002	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.76	J/molxK	812.92	Joback Method
cpg	856.54	J/molxK	978.89	Joback Method
cpg	845.54	J/molxK	945.70	Joback Method
cpg	833.48	J/molxK	912.50	Joback Method
cpg	820.33	J/molxK	879.31	Joback Method
cpg	806.10	J/molxK	846.11	Joback Method
cpg	866.47	J/molxK	1012.09	Joback Method
dvisc	0.0000539	Paxs	812.92	Joback Method

dvisc	0.0000697	Paxs	758.37	Joback Method
dvisc	0.0000937	Paxs	703.81	Joback Method
dvisc	0.0001324	Paxs	649.25	Joback Method
dvisc	0.0001994	Paxs	594.70	Joback Method
dvisc	0.0003262	Paxs	540.14	Joback Method
dvisc	0.0005959	Paxs	485.59	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382173&Units=SI

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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