

Diglycolic acid, hexyl 3-phenylpropyl ester

Inchi:	InChI=1S/C19H28O5/c1-2-3-4-8-13-23-18(20)15-22-16-19(21)24-14-9-12-17-10-6-5-7-1
InchiKey:	YBHKCMJGRHGVQK-UHFFFAOYSA-N
Formula:	C19H28O5
SMILES:	CCCCCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	336.42

Physical Properties

Property code	Value	Unit	Source
gf	-351.33	kJ/mol	Joback Method
hf	-820.78	kJ/mol	Joback Method
hfus	45.77	kJ/mol	Joback Method
hvap	80.89	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.302		Crippen Method
mvol	275.560	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	3148.00		NIST Webbook
tb	835.80	K	Joback Method
tc	1035.35	K	Joback Method
tf	496.86	K	Joback Method
vc	1.058	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.89	J/molxK	835.80	Joback Method
cpg	864.43	J/molxK	869.06	Joback Method
cpg	878.82	J/molxK	902.32	Joback Method
cpg	892.08	J/molxK	935.58	Joback Method
cpg	904.21	J/molxK	968.84	Joback Method
cpg	915.23	J/molxK	1002.09	Joback Method
cpg	925.15	J/molxK	1035.35	Joback Method
dvisc	0.0005380	Paxs	496.86	Joback Method
dvisc	0.0002909	Paxs	553.35	Joback Method

dvisc	0.0001763	Paxs	609.84	Joback Method
dvisc	0.0001163	Paxs	666.33	Joback Method
dvisc	0.0000819	Paxs	722.82	Joback Method
dvisc	0.0000607	Paxs	779.31	Joback Method
dvisc	0.0000468	Paxs	835.80	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=U382175&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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