

Diglycolic acid, ethyl 3-phenylpropyl ester

Inchi:	InChI=1S/C15H20O5/c1-2-19-14(16)11-18-12-15(17)20-10-6-9-13-7-4-3-5-8-13/h3-5,7-8
InchiKey:	BWTDHSIPMPDHEY-UHFFFAOYSA-N
Formula:	C15H20O5
SMILES:	CCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	280.32

Physical Properties

Property code	Value	Unit	Source
gf	-385.01	kJ/mol	Joback Method
hf	-738.22	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	71.98	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.742		Crippen Method
mvol	219.200	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	744.28	K	Joback Method
tc	945.99	K	Joback Method
tf	451.78	K	Joback Method
vc	0.834	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.80	J/molxK	744.28	Joback Method
cpg	684.87	J/molxK	912.37	Joback Method
cpg	674.18	J/molxK	878.75	Joback Method
cpg	662.54	J/molxK	845.14	Joback Method
cpg	649.93	J/molxK	811.52	Joback Method
cpg	636.35	J/molxK	777.90	Joback Method
cpg	694.59	J/molxK	945.99	Joback Method
dvisc	0.0000809	Paxs	744.28	Joback Method

dvisc	0.0001035	Paxs	695.53	Joback Method
dvisc	0.0001375	Paxs	646.78	Joback Method
dvisc	0.0001911	Paxs	598.03	Joback Method
dvisc	0.0002818	Paxs	549.28	Joback Method
dvisc	0.0004480	Paxs	500.53	Joback Method
dvisc	0.0007872	Paxs	451.78	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=U382169&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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