

Diglycolic acid, ethyl 3-methylphenyl ester

Inchi:	InChI=1S/C13H16O5/c1-3-17-12(14)8-16-9-13(15)18-11-6-4-5-10(2)7-11/h4-7H,3,8-9H2
InchiKey:	WYAAFNVMSGFFU-UHFFFAOYSA-N
Formula:	C13H16O5
SMILES:	CCOC(=O)COCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	252.26

Physical Properties

Property code	Value	Unit	Source
gf	-411.48	kJ/mol	Joback Method
hf	-708.41	kJ/mol	Joback Method
hfus	29.84	kJ/mol	Joback Method
hvap	68.19	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.480		Crippen Method
mvol	191.020	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	2269.00		NIST Webbook
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tb	703.50	K	Joback Method
tc	910.34	K	Joback Method
tf	441.76	K	Joback Method
vc	0.722	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.53	J/molxK	703.50	Joback Method
cpg	527.16	J/molxK	737.97	Joback Method
cpg	539.94	J/molxK	772.45	Joback Method
cpg	551.84	J/molxK	806.92	Joback Method
cpg	562.86	J/molxK	841.39	Joback Method
cpg	573.00	J/molxK	875.86	Joback Method
cpg	582.24	J/molxK	910.34	Joback Method
dvisc	0.0007681	Paxs	441.76	Joback Method

dvisc	0.0004738	Paxs	485.38	Joback Method
dvisc	0.0003164	Paxs	529.01	Joback Method
dvisc	0.0002248	Paxs	572.63	Joback Method
dvisc	0.0001676	Paxs	616.25	Joback Method
dvisc	0.0001299	Paxs	659.88	Joback Method
dvisc	0.0001039	Paxs	703.50	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=U382097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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