Diglycolic acid, isobutyl 2-methoxyphenyl ester

Inchi: InChI=1S/C15H20O6/c1-11(2)8-20-14(16)9-19-10-15(17)21-13-7-5-4-6-12(13)18-3/h4-7,

InchiKey: ZGASQFPKBVTPGX-UHFFFAOYSA-N

Formula: C15H20O6

SMILES: COc1ccccc1OC(=O)COCC(=O)OCC(C)C

Mol. weight [g/mol]: 296.32

Physical Properties

Property code	Value	Unit	Source
gf	-502.08	kJ/mol	Joback Method
hf	-887.19	kJ/mol	Joback Method
hfus	32.68	kJ/mol	Joback Method
hvap	74.67	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.816		Crippen Method
mcvol	225.070	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
tb	771.24	K	Joback Method
tc	975.76	K	Joback Method
tf	471.53	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.82	J/mol×K	771.24	Joback Method
cpg	709.63	J/mol×K	941.67	Joback Method
cpg	699.61	J/mol×K	907.59	Joback Method
cpg	688.51	J/mol×K	873.50	Joback Method
cpg	676.33	J/mol×K	839.41	Joback Method
cpg	663.09	J/mol×K	805.33	Joback Method
cpg	718.55	J/mol×K	975.76	Joback Method
dvisc	0.0000569	Pa×s	771.24	Joback Method

dvisc	0.0000727	Pa×s	721.29	Joback Method
dvisc	0.0000962	Pa×s	671.34	Joback Method
dvisc	0.0001334	Pa×s	621.38	Joback Method
dvisc	0.0001956	Pa×s	571.43	Joback Method
dvisc	0.0003088	Pa×s	521.48	Joback Method
dvisc	0.0005370	Pa×s	471.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U382241&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