

Diglycolic acid, isobutyl 4-methoxyphenyl ester

Inchi:	InChI=1S/C15H20O6/c1-11(2)8-20-14(16)9-19-10-15(17)21-13-6-4-12(18-3)5-7-13/h4-7,
InchiKey:	YPRNQBQCGYPSII-UHFFFAOYSA-N
Formula:	C15H20O6
SMILES:	COc1ccc(OC(=O)COCC(=O)OCC(C)C)cc1
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
rinpola	2673.00		NIST Webbook
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tb	771.24	K	Joback Method
tc	975.76	K	Joback Method
tf	471.53	K	Joback Method
vc	0.846	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.82	J/molxK	771.24	Joback Method
cpg	663.09	J/molxK	805.33	Joback Method
cpg	676.33	J/molxK	839.41	Joback Method
cpg	688.51	J/molxK	873.50	Joback Method
cpg	699.61	J/molxK	907.59	Joback Method
cpg	709.63	J/molxK	941.67	Joback Method
cpg	718.55	J/molxK	975.76	Joback Method
dvisc	0.0005370	Paxs	471.53	Joback Method

dvisc	0.0003088	Paxs	521.48	Joback Method
dvisc	0.0001956	Paxs	571.43	Joback Method
dvisc	0.0001334	Paxs	621.38	Joback Method
dvisc	0.0000962	Paxs	671.34	Joback Method
dvisc	0.0000727	Paxs	721.29	Joback Method
dvisc	0.0000569	Paxs	771.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381884&Units=SI
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

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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