

Diglycolic acid, butyl 2-methoxyphenyl ester

Inchi:	InChI=1S/C15H20O6/c1-3-4-9-20-14(16)10-19-11-15(17)21-13-8-6-5-7-12(13)18-2/h5-8H
InchiKey:	BTSYSLNHXAEWJY-UHFFFAOYSA-N
Formula:	C15H20O6
SMILES:	CCCCOC(=O)COCC(=O)Oc1ccccc1OC
Mol. weight [g/mol]:	296.32

Physical Properties

Property code	Value	Unit	Source
gf	-499.64	kJ/mol	Joback Method
hf	-881.91	kJ/mol	Joback Method
hfus	36.21	kJ/mol	Joback Method
hvap	75.05	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.960		Crippen Method
mvol	225.070	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2662.00		NIST Webbook
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tb	771.68	K	Joback Method
tc	973.46	K	Joback Method
tf	486.53	K	Joback Method
vc	0.852	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.26	J/molxK	771.68	Joback Method
cpg	662.34	J/molxK	805.31	Joback Method
cpg	675.41	J/molxK	838.94	Joback Method
cpg	687.47	J/molxK	872.57	Joback Method
cpg	698.50	J/molxK	906.20	Joback Method
cpg	708.48	J/molxK	939.83	Joback Method
cpg	717.39	J/molxK	973.46	Joback Method
dvisc	0.0004754	Paxs	486.53	Joback Method

dvisc	0.0002909	Paxs	534.06	Joback Method
dvisc	0.0001929	Paxs	581.58	Joback Method
dvisc	0.0001361	Paxs	629.11	Joback Method
dvisc	0.0001008	Paxs	676.63	Joback Method
dvisc	0.0000777	Paxs	724.16	Joback Method
dvisc	0.0000618	Paxs	771.68	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=U382242&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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