Diglycolic acid, isobutyl 3-methylphenyl ester

Inchi: InChI=1S/C15H20O5/c1-11(2)8-19-14(16)9-18-10-15(17)20-13-6-4-5-12(3)7-13/h4-7,11H
InchiKey: ZEFVMMQHPLRAIP-UHFFFAOYSA-N
Formula: C15H20O5
SMILES: Cc1cccc(OC(=O)COCC(=O)OCC(C)C)c1
Mol. weight [g/mol]: 280.32

Physical Properties

Property code	Value	Unit	Source
gf	-397.08	kJ/mol	Joback Method
hf	-754.97	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	72.26	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.116		Crippen Method
mcvol	219.200	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
tb	748.82	K	Joback Method
tc	954.33	K	Joback Method
tf	449.30	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.47	J/mol×K	748.82	Joback Method
cpg	636.13	J/mol×K	783.07	Joback Method
cpg	649.79	J/mol×K	817.32	Joback Method
cpg	662.46	J/mol×K	851.57	Joback Method
cpg	674.12	J/mol×K	885.82	Joback Method
cpg	684.78	J/mol×K	920.08	Joback Method
cpg	694.42	J/mol×K	954.33	Joback Method
dvisc	0.0007579	Pa×s	449.30	Joback Method

dvisc	0.0004248	Pa×s	499.22	Joback Method
dvisc	0.0002645	Pa×s	549.14	Joback Method
dvisc	0.0001782	Pa×s	599.06	Joback Method
dvisc	0.0001276	Pa×s	648.98	Joback Method
dvisc	0.0000958	Pa×s	698.90	Joback Method
dvisc	0.0000748	Pa×s	748.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382099&Units=SI
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

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