Diglycolic acid, butyl 3-methylphenyl ester

Inchi: InChI=1S/C15H20O5/c1-3-4-8-19-14(16)10-18-11-15(17)20-13-7-5-6-12(2)9-13/h5-7,9H,
InchiKey: PBHNSVMNNWCRBX-UHFFFAOYSA-N
Formula: C15H20O5
SMILES: CCCCOC(=O)COCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 280.32

Physical Properties

Property code	Value	Unit	Source
gf	-394.64	kJ/mol	Joback Method
hf	-749.69	kJ/mol	Joback Method
hfus	35.02	kJ/mol	Joback Method
hvap	72.64	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.260		Crippen Method
mcvol	219.200	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	749.26	K	Joback Method
tc	951.78	K	Joback Method
tf	464.30	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.91	J/mol×K	749.26	Joback Method
cpg	635.35	J/mol×K	783.01	Joback Method
cpg	648.83	J/mol×K	816.77	Joback Method
cpg	661.35	J/mol×K	850.52	Joback Method
cpg	672.91	J/mol×K	884.27	Joback Method
cpg	683.50	J/mol×K	918.02	Joback Method
cpg	693.12	J/mol×K	951.78	Joback Method
dvisc	0.0006625	Pa×s	464.30	Joback Method

dvisc	0.0003969	Pa×s	511.79	Joback Method
dvisc	0.0002594	Pa×s	559.29	Joback Method
dvisc	0.0001812	Pa×s	606.78	Joback Method
dvisc	0.0001333	Pa×s	654.27	Joback Method
dvisc	0.0001023	Pa×s	701.77	Joback Method
dvisc	0.0000811	Pa×s	749.26	Joback Method

Sources

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=U382100&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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