Diglycolic acid, butyl 2,5-dimethylphenyl ester

Inchi: InChI=1S/C16H22O5/c1-4-5-8-20-15(17)10-19-11-16(18)21-14-9-12(2)6-7-13(14)3/h6-7,
InchiKey: QJJKCMWCTOAZJW-UHFFFAOYSA-N
Formula: C16H22O5
SMILES: CCCCOC(=O)COCC(=O)Oc1cc(C)ccc1C
Mol. weight [g/mol]: 294.34

Physical Properties

Property code	Value	Unit	Source
gf	-395.85	kJ/mol	Joback Method
hf	-781.80	kJ/mol	Joback Method
hfus	37.22	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.569		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2579.00		NIST Webbook
rinpol	2579.00		NIST Webbook
tb	777.12	K	Joback Method
tc	979.03	K	Joback Method
tf	488.09	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.43	J/mol×K	777.12	Joback Method
cpg	690.08	J/mol×K	810.77	Joback Method
cpg	703.73	J/mol×K	844.42	Joback Method
cpg	716.39	J/mol×K	878.08	Joback Method
cpg	728.03	J/mol×K	911.73	Joback Method
cpg	738.65	J/mol×K	945.38	Joback Method
cpg	748.25	J/mol×K	979.03	Joback Method
dvisc	0.0005225	Pa×s	488.09	Joback Method

dvisc	0.0003234	Pa×s	536.26	Joback Method
dvisc	0.0002166	Pa×s	584.43	Joback Method
dvisc	0.0001543	Pa×s	632.61	Joback Method
dvisc	0.0001152	Pa×s	680.78	Joback Method
dvisc	0.0000895	Pa×s	728.95	Joback Method
dvisc	0.0000717	Pa×s	777.12	Joback Method

Sources

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=U382705&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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