Diglycolic acid, 2-formylphenyl propyl ester

Inchi: InChI=1S/C14H16O6/c1-2-7-19-13(16)9-18-10-14(17)20-12-6-4-3-5-11(12)8-15/h3-6,8H,
InchiKey: XUGQXIRHBIWZCA-UHFFFAOYSA-N
Formula: C14H16O6
SMILES: CCCOC(=O)COCC(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 280.27

Physical Properties

Property code	Value	Unit	Source
gf	-502.58	kJ/mol	Joback Method
hf	-814.63	kJ/mol	Joback Method
hfus	34.72	kJ/mol	Joback Method
hvap	77.14	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.374		Crippen Method
mcvol	206.680	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	2580.00		NIST Webbook
rinpol	2580.00		NIST Webbook
tb	775.04	K	Joback Method
tc	982.45	K	Joback Method
tf	495.03	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.29	J/mol×K	775.04	Joback Method
cpg	593.61	J/mol×K	809.61	Joback Method
cpg	604.98	J/mol×K	844.18	Joback Method
cpg	615.40	J/mol×K	878.75	Joback Method
cpg	624.87	J/mol×K	913.31	Joback Method
cpg	633.37	J/mol×K	947.88	Joback Method
cpg	640.90	J/mol×K	982.45	Joback Method
dvisc	0.0007041	Pa×s	495.03	Joback Method

dvisc	0.0004430	Pa×s	541.70	Joback Method
dvisc	0.0003000	Pa×s	588.37	Joback Method
dvisc	0.0002152	Pa×s	635.03	Joback Method
dvisc	0.0001615	Pa×s	681.70	Joback Method
dvisc	0.0001257	Pa×s	728.37	Joback Method
dvisc	0.0001009	Pa×s	775.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382307&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