Diglycolic acid, 2-formylphenyl isobutyl ester

Inchi: InChI=1S/C15H18O6/c1-11(2)8-20-14(17)9-19-10-15(18)21-13-6-4-3-5-12(13)7-16/h3-7,
InchiKey: XFRVGBCOERRDTE-UHFFFAOYSA-N
Formula: C15H18O6
SMILES: CC(C)COC(=O)COCC(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 294.30

Physical Properties

Property code	Value	Unit	Source
gf	-496.60	kJ/mol	Joback Method
hf	-840.55	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	78.98	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.620		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	2648.00		NIST Webbook
tb	797.48	K	Joback Method
tc	1006.12	K	Joback Method
tf	491.30	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.43	J/mol×K	797.48	Joback Method
cpg	690.13	J/mol×K	971.35	Joback Method
cpg	681.46	J/mol×K	936.58	Joback Method
cpg	671.76	J/mol×K	901.80	Joback Method
cpg	661.01	J/mol×K	867.03	Joback Method
cpg	649.24	J/mol×K	832.25	Joback Method
cpg	697.75	J/mol×K	1006.12	Joback Method
dvisc	0.0000814	Pa×s	797.48	Joback Method
dvisc	0.0001034	Pa×s	746.45	Joback Method

dvisc	0.0001360	Pa×s	695.42	Joback Method
dvisc	0.0001870	Pa×s	644.39	Joback Method
dvisc	0.0002715	Pa×s	593.36	Joback Method
dvisc	0.0004229	Pa×s	542.33	Joback Method
dvisc	0.0007222	Pa×s	491.30	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=U382308&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