Diglycolic acid, 2-formylphenyl pentyl ester

Inchi: InChI=1S/C16H20O6/c1-2-3-6-9-21-15(18)11-20-12-16(19)22-14-8-5-4-7-13(14)10-17/h4
InchiKey: OMNXZWWODTURCN-UHFFFAOYSA-N
Formula: C16H20O6
SMILES: CCCCCOC(=O)COCC(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 308.33

Physical Properties

Property code	Value	Unit	Source
gf	-485.74	kJ/mol	Joback Method
hf	-855.91	kJ/mol	Joback Method
hfus	39.90	kJ/mol	Joback Method
hvap	81.59	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.154		Crippen Method
mcvol	234.860	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	2835.00		NIST Webbook
rinpol	2835.00		NIST Webbook
tb	820.80	K	Joback Method
tc	1025.89	K	Joback Method
tf	517.57	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.39	J/mol×K	820.80	Joback Method
cpg	704.31	J/mol×K	854.98	Joback Method
cpg	716.19	J/mol×K	889.16	Joback Method
cpg	727.03	J/mol×K	923.34	Joback Method
cpg	736.82	J/mol×K	957.52	Joback Method
cpg	745.57	J/mol×K	991.71	Joback Method
cpg	753.27	J/mol×K	1025.89	Joback Method
dvisc	0.0005923	Pa×s	517.57	Joback Method

dvisc	0.0003629	Pa×s	568.11	Joback Method
dvisc	0.0002409	Pa×s	618.65	Joback Method
dvisc	0.0001701	Pa×s	669.18	Joback Method
dvisc	0.0001261	Pa×s	719.72	Joback Method
dvisc	0.0000973	Pa×s	770.26	Joback Method
dvisc	0.0000774	Pa×s	820.80	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382310&Units=SI

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