Diglycolic acid, 2-isopropylphenyl pentyl ester

Inchi: InChI=1S/C18H26O5/c1-4-5-8-11-22-17(19)12-21-13-18(20)23-16-10-7-6-9-15(16)14(2)3
InchiKey: QREZTYLBQIDPGF-UHFFFAOYSA-N
Formula: C18H26O5
SMILES: CCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-371.82	kJ/mol	Joback Method
hf	-816.89	kJ/mol	Joback Method
hfus	39.27	kJ/mol	Joback Method
hvap	78.93	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.465		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tb	817.46	K	Joback Method
tc	1019.56	K	Joback Method
tf	483.11	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.54	J/mol×K	817.46	Joback Method
cpg	856.24	J/mol×K	985.88	Joback Method
cpg	845.35	J/mol×K	952.19	Joback Method
cpg	833.34	J/mol×K	918.51	Joback Method
cpg	820.20	J/mol×K	884.83	Joback Method
cpg	805.94	J/mol×K	851.14	Joback Method
cpg	866.02	J/mol×K	1019.56	Joback Method
dvisc	0.0000500	Pa×s	817.46	Joback Method

dvisc	0.0000647	Pa×s	761.73	Joback Method
dvisc	0.0000872	Pa×s	706.01	Joback Method
dvisc	0.0001237	Pa×s	650.28	Joback Method
dvisc	0.0001875	Pa×s	594.56	Joback Method
dvisc	0.0003097	Pa×s	538.84	Joback Method
dvisc	0.0005741	Pa×s	483.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382289&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