Diglycolic acid, di(2-isopropoxyphenyl) ester

Inchi: InChI=1S/C22H26O7/c1-15(2)26-17-9-5-7-11-19(17)28-21(23)13-25-14-22(24)29-20-12-
InchiKey: ARZKOGPKYTVUTN-UHFFFAOYSA-N
Formula: C22H26O7
SMILES: CC(C)Oc1ccccc1OC(=O)COCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 402.44

Physical Properties

Property code	Value	Unit	Source
gf	-447.80	kJ/mol	Joback Method
hf	-944.11	kJ/mol	Joback Method
hfus	42.13	kJ/mol	Joback Method
hvap	95.21	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.789		Crippen Method
mcvol	305.810	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	3540.00		NIST Webbook
rinpol	3540.00		NIST Webbook
tb	985.04	K	Joback Method
tc	1213.82	K	Joback Method
tf	596.59	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.15	J/mol×K	985.04	Joback Method
cpg	989.47	J/mol×K	1023.17	Joback Method
cpg	998.94	J/mol×K	1061.30	Joback Method
cpg	1006.52	J/mol×K	1099.43	Joback Method
cpg	1012.21	J/mol×K	1137.56	Joback Method
cpg	1015.99	J/mol×K	1175.69	Joback Method
cpg	1017.85	J/mol×K	1213.82	Joback Method
dvisc	0.0001516	Pa×s	596.59	Joback Method

dvisc	0.0000850	Pa×s	661.33	Joback Method
dvisc	0.0000529	Pa×s	726.07	Joback Method
dvisc	0.0000355	Pa×s	790.82	Joback Method
dvisc	0.0000254	Pa×s	855.56	Joback Method
dvisc	0.0000190	Pa×s	920.30	Joback Method
dvisc	0.0000148	Pa×s	985.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381983&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

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