Diglycolic acid, di(2-isopropylphenyl) ester

Inchi: InChI=1S/C22H26O5/c1-15(2)17-9-5-7-11-19(17)26-21(23)13-25-14-22(24)27-20-12-8-6
InchiKey: UZAPBJLVRRZRNM-UHFFFAOYSA-N
Formula: C22H26O5
SMILES: CC(C)c1ccccc1OC(=O)COCC(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]: 370.44

Physical Properties

Property code	Value	Unit	Source
gf	-237.80	kJ/mol	Joback Method
hf	-679.67	kJ/mol	Joback Method
hfus	39.76	kJ/mol	Joback Method
hvap	90.39	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.461		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	3157.00		NIST Webbook
rinpol	3157.00		NIST Webbook
tb	940.20	K	Joback Method
tc	1167.22	K	Joback Method
tf	552.13	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.14	J/mol×K	940.20	Joback Method
cpg	938.67	J/mol×K	978.04	Joback Method
cpg	950.66	J/mol×K	1015.87	Joback Method
cpg	961.13	J/mol×K	1053.71	Joback Method
cpg	970.11	J/mol×K	1091.54	Joback Method
cpg	977.62	J/mol×K	1129.38	Joback Method
cpg	983.68	J/mol×K	1167.22	Joback Method
dvisc	0.0003123	Pa×s	552.13	Joback Method

dvisc	0.0001675	Pa×s	616.81	Joback Method
dvisc	0.0001011	Pa×s	681.49	Joback Method
dvisc	0.0000666	Pa×s	746.16	Joback Method
dvisc	0.0000469	Pa×s	810.84	Joback Method
dvisc	0.0000348	Pa×s	875.52	Joback Method
dvisc	0.0000269	Pa×s	940.20	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=U382294&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