Isophthalic acid, di(1-isopropyl-2-methylpropyl) ester

Inchi: InChI=1S/C22H34O4/c1-13(2)19(14(3)4)25-21(23)17-10-9-11-18(12-17)22(24)26-20(15(

InchiKey: OVNLBUVYWFGXSX-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CC(C)C(OC(=O)c1cccc(C(=O)OC(C(C)C)C(C)C)c1)C(C)C

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-245.34	kJ/mol	Joback Method
hf	-793.63	kJ/mol	Joback Method
hfus	30.82	kJ/mol	Joback Method
hvap	83.49	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.361		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook
tb	884.36	K	Joback Method
tc	1096.21	K	Joback Method
tf	430.96	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.18	J/mol×K	884.36	Joback Method
cpg	1017.29	J/mol×K	919.67	Joback Method
cpg	1033.00	J/mol×K	954.98	Joback Method
cpg	1047.32	J/mol×K	990.28	Joback Method
cpg	1060.31	J/mol×K	1025.59	Joback Method
cpg	1071.98	J/mol×K	1060.90	Joback Method
cpg	1082.37	J/mol×K	1096.21	Joback Method
dvisc	0.0012639	Pa×s	430.96	Joback Method

dvisc	0.0003994	Pa×s	506.53	Joback Method
dvisc	0.0001702	Pa×s	582.09	Joback Method
dvisc	0.0000883	Pa×s	657.66	Joback Method
dvisc	0.0000524	Pa×s	733.23	Joback Method
dvisc	0.0000343	Pa×s	808.79	Joback Method
dvisc	0.0000241	Pa×s	884.36	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=U356372&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