Isophthalic acid, isohexyl 1-isopropyl-2-methylpropyl ester

Inchi: InChI=1S/C21H32O4/c1-14(2)9-8-12-24-20(22)17-10-7-11-18(13-17)21(23)25-19(15(3)4

InchiKey: DQEXJHJXRBVXAG-UHFFFAOYSA-N

Formula: C21H32O4

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

Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-248.88	kJ/mol	Joback Method
hf	-762.43	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	82.04	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.117		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	862.36	K	Joback Method
tc	1070.10	K	Joback Method
tf	449.69	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.16	J/mol×K	862.36	Joback Method
cpg	955.95	J/mol×K	896.98	Joback Method
cpg	971.45	J/mol×K	931.61	Joback Method
cpg	985.68	J/mol×K	966.23	Joback Method
cpg	998.67	J/mol×K	1000.86	Joback Method
cpg	1010.44	J/mol×K	1035.48	Joback Method
cpg	1021.02	J/mol×K	1070.10	Joback Method
dvisc	0.0009632	Pa×s	449.69	Joback Method

dvisc	0.0003795	Pa×s	518.47	Joback Method
dvisc	0.0001859	Pa×s	587.25	Joback Method
dvisc	0.0001058	Pa×s	656.02	Joback Method
dvisc	0.0000670	Pa×s	724.80	Joback Method
dvisc	0.0000459	Pa×s	793.58	Joback Method
dvisc	0.0000334	Pa×s	862.36	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=U356371&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