Isophthalic acid, isohexyl 2-isopropylphenyl ester

Inchi: InChI=1S/C23H28O4/c1-16(2)9-8-14-26-22(24)18-10-7-11-19(15-18)23(25)27-21-13-6-5

InchiKey: YYYIYIINSDMEGK-UHFFFAOYSA-N

Formula: C23H28O4

SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2ccccc2C(C)C)c1

Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-124.38	kJ/mol	Joback Method
hf	-568.09	kJ/mol	Joback Method
hfus	41.16	kJ/mol	Joback Method
hvap	90.20	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.622		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	940.66	K	Joback Method
tc	1167.15	K	Joback Method
tf	541.17	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.88	J/mol×K	940.66	Joback Method
cpg	971.30	J/mol×K	978.41	Joback Method
cpg	984.28	J/mol×K	1016.16	Joback Method
cpg	995.86	J/mol×K	1053.90	Joback Method
cpg	1006.09	J/mol×K	1091.65	Joback Method
cpg	1015.00	J/mol×K	1129.40	Joback Method
cpg	1022.64	J/mol×K	1167.15	Joback Method
dvisc	0.0004011	Pa×s	541.17	Joback Method

dvisc	0.0002076	Pa×s	607.75	Joback Method
dvisc	0.0001224	Pa×s	674.33	Joback Method
dvisc	0.0000794	Pa×s	740.91	Joback Method
dvisc	0.0000553	Pa×s	807.50	Joback Method
dvisc	0.0000407	Pa×s	874.08	Joback Method
dvisc	0.0000312	Pa×s	940.66	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=U344635&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