

Isophthalic acid, isohexyl 2-methylcyclohexyl ester

Inchi:	InChI=1S/C21H30O4/c1-15(2)8-7-13-24-20(22)17-10-6-11-18(14-17)21(23)25-19-12-5-4
InchiKey:	BZIQKXGWONQDKW-UHFFFAOYSA-N
Formula:	C21H30O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1
Mol. weight [g/mol]:	346.46

Physical Properties

Property code	Value	Unit	Source
gf	-224.82	kJ/mol	Joback Method
hf	-712.61	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	83.32	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.015		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	2613.00		NIST Webbook
rinpol	2613.00		NIST Webbook
tb	878.56	K	Joback Method
tc	1098.94	K	Joback Method
tf	497.83	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.00	J/molxK	878.56	Joback Method
cpg	1008.23	J/molxK	1062.21	Joback Method
cpg	997.10	J/molxK	1025.48	Joback Method
cpg	984.44	J/molxK	988.75	Joback Method
cpg	970.22	J/molxK	952.02	Joback Method
cpg	954.42	J/molxK	915.29	Joback Method
cpg	1017.85	J/molxK	1098.94	Joback Method
dvisc	0.0000587	Paxs	878.56	Joback Method

dvisc	0.0000761	Paxs	815.11	Joback Method
dvisc	0.0001030	Paxs	751.65	Joback Method
dvisc	0.0001473	Paxs	688.19	Joback Method
dvisc	0.0002267	Paxs	624.74	Joback Method
dvisc	0.0003846	Paxs	561.28	Joback Method
dvisc	0.0007467	Paxs	497.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U345750&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

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