

Isophthalic acid, isohexyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C20H30O4/c1-14(2)8-7-11-23-19(21)17-9-6-10-18(13-17)20(22)24-16(5)12-15
InchiKey:	WNESSKNIHAVGCG-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-254.86	kJ/mol	Joback Method
hf	-736.51	kJ/mol	Joback Method
hfus	36.21	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.871		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1365.67	kPa	Joback Method
rinsol	2263.00		NIST Webbook
tb	839.92	K	Joback Method
tc	1045.58	K	Joback Method
tf	453.42	K	Joback Method
vc	1.077	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.27	J/molxK	839.92	Joback Method
cpg	950.00	J/molxK	1011.30	Joback Method
cpg	938.21	J/molxK	977.03	Joback Method
cpg	925.26	J/molxK	942.75	Joback Method
cpg	911.14	J/molxK	908.47	Joback Method
cpg	895.82	J/molxK	874.20	Joback Method
cpg	960.66	J/molxK	1045.58	Joback Method
dvisc	0.0000422	Paxs	839.92	Joback Method
dvisc	0.0000569	Paxs	775.50	Joback Method

dvisc	0.0000811	Paxs	711.09	Joback Method
dvisc	0.0001239	Paxs	646.67	Joback Method
dvisc	0.0002078	Paxs	582.25	Joback Method
dvisc	0.0003967	Paxs	517.84	Joback Method
dvisc	0.0009099	Paxs	453.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356442&Units=SI
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

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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