

Isophthalic acid, isohexyl neopentyl ester

Inchi:	InChI=1S/C19H28O4/c1-14(2)8-7-11-22-17(20)15-9-6-10-16(12-15)18(21)23-13-19(3,4)5
InchiKey:	NWBFXIMOOYELGJ-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-255.56	kJ/mol	Joback Method
hf	-714.06	kJ/mol	Joback Method
hfus	33.25	kJ/mol	Joback Method
hvap	77.45	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.482		Crippen Method
mvol	269.690	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	2262.00		NIST Webbook
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tb	814.69	K	Joback Method
tc	1022.76	K	Joback Method
tf	474.57	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.88	J/molxK	814.69	Joback Method
cpg	837.19	J/molxK	849.37	Joback Method
cpg	852.34	J/molxK	884.05	Joback Method
cpg	866.36	J/molxK	918.73	Joback Method
cpg	879.29	J/molxK	953.41	Joback Method
cpg	891.18	J/molxK	988.09	Joback Method
cpg	902.07	J/molxK	1022.76	Joback Method
dvisc	0.0007029	Paxs	474.57	Joback Method

dvisc	0.0003503	Paxs	531.26	Joback Method
dvisc	0.0001997	Paxs	587.94	Joback Method
dvisc	0.0001257	Paxs	644.63	Joback Method
dvisc	0.0000852	Paxs	701.32	Joback Method
dvisc	0.0000613	Paxs	758.00	Joback Method
dvisc	0.0000461	Paxs	814.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343863&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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