

Isophthalic acid, isohexyl 1-naphthyl ester

Inchi:	InChI=1S/C24H24O4/c1-17(2)8-7-15-27-23(25)19-11-5-12-20(16-19)24(26)28-22-14-6-1
InchiKey:	XQIVTXAUQWDSGD-UHFFFAOYSA-N
Formula:	C24H24O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)Oc2cccc3ccccc23)c1
Mol. weight [g/mol]:	376.44

Physical Properties

Property code	Value	Unit	Source
gf	-6.87	kJ/mol	Joback Method
hf	-392.38	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	94.46	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	5.652		Crippen Method
mvol	296.920	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	3241.00		NIST Webbook
rinpol	3241.00		NIST Webbook
tb	982.96	K	Joback Method
tc	1221.48	K	Joback Method
tf	600.14	K	Joback Method
vc	1.127	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.41	J/molxK	982.96	Joback Method
cpg	946.49	J/molxK	1022.71	Joback Method
cpg	958.33	J/molxK	1062.47	Joback Method
cpg	969.03	J/molxK	1102.22	Joback Method
cpg	978.67	J/molxK	1141.97	Joback Method
cpg	987.34	J/molxK	1181.73	Joback Method
cpg	995.12	J/molxK	1221.48	Joback Method
dvisc	0.0004371	Paxs	600.14	Joback Method

dvisc	0.0002699	Paxs	663.94	Joback Method
dvisc	0.0001813	Paxs	727.75	Joback Method
dvisc	0.0001299	Paxs	791.55	Joback Method
dvisc	0.0000978	Paxs	855.35	Joback Method
dvisc	0.0000766	Paxs	919.16	Joback Method
dvisc	0.0000619	Paxs	982.96	Joback Method

Sources

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=U344689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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