

Isophthalic acid, hexyl 1-naphthyl ester

Inchi:	InChI=1S/C24H24O4/c1-2-3-4-7-16-27-23(25)19-12-8-13-20(17-19)24(26)28-22-15-9-11
InchiKey:	IIMJKKDGMLRAOY-UHFFFAOYSA-N
Formula:	C24H24O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2cccc3ccccc23)c1
Mol. weight [g/mol]:	376.44

Physical Properties

Property code	Value	Unit	Source
gf	-4.43	kJ/mol	Joback Method
hf	-387.10	kJ/mol	Joback Method
hfus	47.81	kJ/mol	Joback Method
hvap	94.85	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	5.796		Crippen Method
mvol	296.920	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	3289.00		NIST Webbook
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tb	983.40	K	Joback Method
tc	1219.68	K	Joback Method
tf	615.14	K	Joback Method
vc	1.133	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.99	J/molxK	983.40	Joback Method
cpg	946.02	J/molxK	1022.78	Joback Method
cpg	957.85	J/molxK	1062.16	Joback Method
cpg	968.57	J/molxK	1101.54	Joback Method
cpg	978.26	J/molxK	1140.92	Joback Method
cpg	987.02	J/molxK	1180.30	Joback Method
cpg	994.92	J/molxK	1219.68	Joback Method
dvisc	0.0004158	Paxs	615.14	Joback Method

dvisc	0.0002682	Paxs	676.52	Joback Method
dvisc	0.0001861	Paxs	737.89	Joback Method
dvisc	0.0001366	Paxs	799.27	Joback Method
dvisc	0.0001047	Paxs	860.65	Joback Method
dvisc	0.0000832	Paxs	922.02	Joback Method
dvisc	0.0000680	Paxs	983.40	Joback Method

Sources

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=U344690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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