

Isophthalic acid, diamide, N,N'-bis(2-ethylhexyl)-

Other names:	Isophthalic acid, diamide, N,N'-(2-ethylhexyl)-
Inchi:	InChI=1S/C24H40N2O2/c1-5-9-12-19(7-3)17-25-23(27)21-14-11-15-22(16-21)24(28)26-
InchiKey:	VYSKTPNDJPCJKY-UHFFFAOYSA-N
Formula:	C24H40N2O2
SMILES:	CCCCC(CC)CNC(=O)c1cccc(C(=O)NCC(CC)CCCC)c1
Mol. weight [g/mol]:	388.59

Physical Properties

Property code	Value	Unit	Source
gf	170.04	kJ/mol	Joback Method
hf	-442.41	kJ/mol	Joback Method
hfus	57.92	kJ/mol	Joback Method
hvap	97.54	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	5.579		Crippen Method
mvol	348.360	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	3437.00		NIST Webbook
rinpol	3437.00		NIST Webbook
tb	987.38	K	Joback Method
tc	1208.92	K	Joback Method
tf	574.36	K	Joback Method
vc	1.341	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.96	J/molxK	987.38	Joback Method
cpg	1199.74	J/molxK	1024.30	Joback Method
cpg	1215.27	J/molxK	1061.23	Joback Method
cpg	1229.63	J/molxK	1098.15	Joback Method
cpg	1242.89	J/molxK	1135.07	Joback Method
cpg	1255.15	J/molxK	1172.00	Joback Method
cpg	1266.48	J/molxK	1208.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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