

Isophthalic acid, diamide, N,N,N',N'-tetrakis(isobutyl)-

Other names: Isophthalic acid, diamide, N,N'-tetrakisobutyl-

Inchi: InChI=1S/C24H40N2O2/c1-17(2)13-25(14-18(3)4)23(27)21-10-9-11-22(12-21)24(28)26(

InchiKey: DKRQMXPAANJJPY-UHFFFAOYSA-N

Formula: C24H40N2O2

SMILES: CC(C)CN(CC(C)C)C(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1

Mol. weight [g/mol]: 388.59

Physical Properties

Property code	Value	Unit	Source
gf	207.94	kJ/mol	Joback Method
hf	-424.85	kJ/mol	Joback Method
hfus	46.72	kJ/mol	Joback Method
hvap	87.98	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.195		Crippen Method
mcvol	348.360	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	2724.00		NIST Webbook
rinpol	2724.00		NIST Webbook
tb	911.04	K	Joback Method
tc	1119.87	K	Joback Method
tf	503.98	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.69	J/molxK	911.04	Joback Method
cpg	1166.05	J/molxK	945.85	Joback Method
cpg	1183.18	J/molxK	980.65	Joback Method
cpg	1199.15	J/molxK	1015.46	Joback Method
cpg	1214.05	J/molxK	1050.26	Joback Method
cpg	1227.96	J/molxK	1085.07	Joback Method
cpg	1240.97	J/molxK	1119.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345806&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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