

Isophthalic acid, monoamide, N,N-diisobutyl-, isohexyl ester

Other names:	Isophthalic acid, monoamide, N-diisobutyl-, isohexyl ester
Inchi:	InChI=1S/C22H35NO3/c1-16(2)9-8-12-26-22(25)20-11-7-10-19(13-20)21(24)23(14-17(3)
InchiKey:	INOODSYHEDROCB-UHFFFAOYSA-N
Formula:	C22H35NO3
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]:	361.52

Physical Properties

Property code	Value	Unit	Source
gf	-22.24	kJ/mol	Joback Method
hf	-578.04	kJ/mol	Joback Method
hfus	43.23	kJ/mol	Joback Method
hvap	84.28	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.034		Crippen Method
mvol	316.070	ml/mol	McGowan Method
pc	1203.12	kPa	Joback Method
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
tb	875.70	K	Joback Method
tc	1081.24	K	Joback Method
tf	486.20	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.74	J/molxK	875.70	Joback Method
cpg	1029.10	J/molxK	909.96	Joback Method
cpg	1045.21	J/molxK	944.21	Joback Method
cpg	1060.14	J/molxK	978.47	Joback Method
cpg	1073.94	J/molxK	1012.73	Joback Method
cpg	1086.66	J/molxK	1046.99	Joback Method
cpg	1098.36	J/molxK	1081.24	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=U345799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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