

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

Other names:	Isophthalic acid, monoamide, N-diisobutyl-, hexyl ester
Inchi:	InChI=1S/C22H35NO3/c1-6-7-8-9-13-26-22(25)20-12-10-11-19(14-20)21(24)23(15-17(2)
InchiKey:	AUQTWUYBYULPFW-UHFFFAOYSA-N
Formula:	C22H35NO3
SMILES:	CCCCCCOC(=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	-19.80	kJ/mol	Joback Method
hf	-572.76	kJ/mol	Joback Method
hfus	46.75	kJ/mol	Joback Method
hvap	84.67	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.178		Crippen Method
mvol	316.070	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	876.14	K	Joback Method
tc	1080.24	K	Joback Method
tf	501.20	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.26	J/molxK	876.14	Joback Method
cpg	1028.51	J/molxK	910.16	Joback Method
cpg	1044.56	J/molxK	944.17	Joback Method
cpg	1059.45	J/molxK	978.19	Joback Method
cpg	1073.23	J/molxK	1012.21	Joback Method
cpg	1085.96	J/molxK	1046.22	Joback Method
cpg	1097.68	J/molxK	1080.24	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U345800&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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