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

Other names: Isophthalic acid, monoamide, N-diisobutyl-, pentyl ester

Inchi: InChI=1S/C21H33NO3/c1-6-7-8-12-25-21(24)19-11-9-10-18(13-19)20(23)22(14-16(2)3)1

InchiKey: MBGMNTHIVRLQGS-UHFFFAOYSA-N

Formula: C21H33NO3

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

Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
gf	-28.22	kJ/mol	Joback Method
hf	-552.12	kJ/mol	Joback Method
hfus	44.16	kJ/mol	Joback Method
hvap	82.45	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.788		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
tb	853.26	K	Joback Method
tc	1056.23	K	Joback Method
tf	489.93	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.02	J/mol×K	853.26	Joback Method
cpg	968.09	J/mol×K	887.09	Joback Method
cpg	983.98	J/mol×K	920.92	Joback Method
cpg	998.75	J/mol×K	954.74	Joback Method
cpg	1012.43	J/mol×K	988.57	Joback Method
cpg	1025.08	J/mol×K	1022.40	Joback Method
cpg	1036.74	J/mol×K	1056.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U345798&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
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
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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