

Isophthalic acid, monoamide, N-butyl-, isobutyl ester

Inchi:	InChI=1S/C16H23NO3/c1-4-5-9-17-15(18)13-7-6-8-14(10-13)16(19)20-11-12(2)3/h6-8,10
InchiKey:	CCNANCYWNHNYMX-UHFFFAOYSA-N
Formula:	C16H23NO3
SMILES:	CCCCNC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]:	277.36

Physical Properties

Property code	Value	Unit	Source
gf	-89.27	kJ/mol	Joback Method
hf	-457.70	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.029		Crippen Method
mvol	231.530	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tb	777.03	K	Joback Method
tc	983.90	K	Joback Method
tf	468.77	K	Joback Method
vc	0.882	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.44	J/molxK	777.03	Joback Method
cpg	692.45	J/molxK	811.51	Joback Method
cpg	706.43	J/molxK	845.99	Joback Method
cpg	719.42	J/molxK	880.46	Joback Method
cpg	731.45	J/molxK	914.94	Joback Method
cpg	742.54	J/molxK	949.42	Joback Method
cpg	752.73	J/molxK	983.90	Joback Method

Sources

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=U345808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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