

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

Inchi:	InChI=1S/C16H23NO3/c1-3-5-10-17-15(18)13-8-7-9-14(12-13)16(19)20-11-6-4-2/h7-9,12
InchiKey:	CDXYABZLCLUGNY-UHFFFAOYSA-N
Formula:	C16H23NO3
SMILES:	CCCCNC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]:	277.36

Physical Properties

Property code	Value	Unit	Source
gf	-86.83	kJ/mol	Joback Method
hf	-452.42	kJ/mol	Joback Method
hfus	40.33	kJ/mol	Joback Method
hvap	76.49	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.173		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	777.47	K	Joback Method
tc	981.54	K	Joback Method
tf	483.77	K	Joback Method
vc	0.888	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.89	J/molxK	777.47	Joback Method
cpg	691.69	J/molxK	811.48	Joback Method
cpg	705.50	J/molxK	845.49	Joback Method
cpg	718.36	J/molxK	879.50	Joback Method
cpg	730.30	J/molxK	913.51	Joback Method
cpg	741.33	J/molxK	947.53	Joback Method
cpg	751.49	J/molxK	981.54	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=U345809&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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