

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

Other names:	Isophthalic acid, monoamide, N-diisobutyl-, butyl ester
Inchi:	InChI=1S/C20H31NO3/c1-6-7-11-24-20(23)18-10-8-9-17(12-18)19(22)21(13-15(2)3)14-1
InchiKey:	PDSIASOLUSOFDC-UHFFFAOYSA-N
Formula:	C20H31NO3
SMILES:	CCCCOC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]:	333.46

Physical Properties

Property code	Value	Unit	Source
gf	-36.64	kJ/mol	Joback Method
hf	-531.48	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	80.22	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.398		Crippen Method
mvol	287.890	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
tb	830.38	K	Joback Method
tc	1032.94	K	Joback Method
tf	478.66	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.50	J/molxK	830.38	Joback Method
cpg	908.40	J/molxK	864.14	Joback Method
cpg	924.15	J/molxK	897.90	Joback Method
cpg	938.79	J/molxK	931.66	Joback Method
cpg	952.37	J/molxK	965.42	Joback Method
cpg	964.93	J/molxK	999.18	Joback Method
cpg	976.52	J/molxK	1032.94	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=U345797&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
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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