

Phthalamide

Other names:	1,2-Benzenedicarboxamide NCI-C03612 NSC 5512 P-D Phthaldiamide Phthalic acid diamide Phthalic diamide o-Carbamoylbenzamide o-Phthalamide o-Phthalic acid diamide
Inchi:	InChI=1S/C8H8N2O2/c9-7(11)5-3-1-2-4-6(5)8(10)12/h1-4H,(H2,9,11)(H2,10,12)
InchiKey:	NAYYNDKKH0I0D-UHFFFAOYSA-N
Formula:	C8H8N2O2
SMILES:	NC(=O)c1ccccc1C(N)=O
Mol. weight [g/mol]:	164.16
CAS:	88-96-0

Physical Properties

Property code	Value	Unit	Source
gf	-5.68	kJ/mol	Joback Method
hf	-140.97	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	71.11	kJ/mol	Joback Method
log10ws	-2.92		Aqueous Solubility Prediction Method
logp	-0.116		Crippen Method
mcpvol	122.920	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	666.90	K	Joback Method
tc	914.95	K	Joback Method
tf	485.24	K	Joback Method
vc	0.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.26	J/mol×K	666.90	Joback Method
cpg	312.95	J/mol×K	708.24	Joback Method
cpg	321.83	J/mol×K	749.58	Joback Method
cpg	329.94	J/mol×K	790.92	Joback Method
cpg	337.31	J/mol×K	832.27	Joback Method
cpg	343.99	J/mol×K	873.61	Joback Method
cpg	350.01	J/mol×K	914.95	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C88960&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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