

3,6-Bis(dimethylamino)phthalimide

Inchi:	InChI=1S/C12H15N3O2/c1-14(2)7-5-6-8(15(3)4)10-9(7)11(16)13-12(10)17/h5-6H,1-4H3,
InchiKey:	DVPKTCEDGEYAOSB-UHFFFAOYSA-N
Formula:	C12H15N3O2
SMILES:	CN(C)c1ccc(N(C)C)c2c1C(=O)NC2=O
Mol. weight [g/mol]:	233.27
CAS:	5972-07-6

Physical Properties

Property code	Value	Unit	Source
gf	266.23	kJ/mol	Joback Method
hf	-98.28	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	0.702		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	736.06	K	Joback Method
tc	975.10	K	Joback Method
tf	617.57	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.51	J/molxK	736.06	Joback Method
cpg	523.81	J/molxK	775.90	Joback Method
cpg	538.00	J/molxK	815.74	Joback Method
cpg	551.08	J/molxK	855.58	Joback Method
cpg	563.07	J/molxK	895.42	Joback Method
cpg	573.97	J/molxK	935.26	Joback Method
cpg	583.79	J/molxK	975.10	Joback Method
hsubt	105.00	kJ/mol	428.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5972076&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hsubt:	Enthalpy of sublimation at a given temperature
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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