

1,7-Diamino-beta-naphthol

Inchi:	InChI=1S/C10H10N2O/c11-7-3-1-6-2-4-9(13)10(12)8(6)5-7/h1-5,13H,11-12H2
InchiKey:	LWYNEQNVMPRDJP-UHFFFAOYSA-N
Formula:	C10H10N2O
SMILES:	Nc1ccc2ccc(O)c(N)c2c1
Mol. weight [g/mol]:	174.20
CAS:	116400-70-5

Physical Properties

Property code	Value	Unit	Source
gf	211.40	kJ/mol	Joback Method
hf	45.20	kJ/mol	Joback Method
hfus	28.11	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.710		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
pc	5335.72	kPa	Joback Method
tb	709.50	K	Joback Method
tc	974.11	K	Joback Method
tf	564.86	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.86	J/mol×K	709.50	Joback Method
cpg	365.06	J/mol×K	753.60	Joback Method
cpg	374.59	J/mol×K	797.70	Joback Method
cpg	383.60	J/mol×K	841.80	Joback Method
cpg	392.26	J/mol×K	885.90	Joback Method
cpg	400.73	J/mol×K	930.01	Joback Method
cpg	409.19	J/mol×K	974.11	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=C116400705&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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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