

1-Naphthalenecarbonitrile, 4-amino-

Other names:	4-Amino-1-naphthalenecarbonitrile 1-Amino-4-cyano naphthalene 4-aminonaphthalene-1-carbonitrile
Inchi:	InChI=1S/C11H8N2/c12-7-8-5-6-11(13)10-4-2-1-3-9(8)10/h1-6H,13H2
InchiKey:	LUSIZUFVMKYWGX-UHFFFAOYSA-N
Formula:	C11H8N2
SMILES:	N#Cc1ccc(N)c2ccccc12
Mol. weight [g/mol]:	168.19
CAS:	58728-64-6

Physical Properties

Property code	Value	Unit	Source
gf	441.17	kJ/mol	Joback Method
hf	332.96	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	66.44	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.294		Crippen Method
mcvol	133.990	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	681.31	K	Joback Method
tc	939.11	K	Joback Method
tf	446.14	K	Joback Method
vc	0.520	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.71	J/mol×K	681.31	Joback Method
cpg	334.01	J/mol×K	724.28	Joback Method
cpg	343.48	J/mol×K	767.24	Joback Method
cpg	352.19	J/mol×K	810.21	Joback Method
cpg	360.24	J/mol×K	853.18	Joback Method
cpg	367.71	J/mol×K	896.15	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=C58728646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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