Naphthalene, 1-isocyano-

Other names: 1-Naphthyl isocyanide
Inchi: InChI=1S/C11H7N/c1-12-11-8-4-6-9-5-2-3-7-10(9)11/h2-8H
InchiKey: PTCSLGONLAYNQB-UHFFFAOYSA-N
Formula: C11H7N
SMILES: [C-]#[N+]c1cccc2ccccc12
Mol. weight [g/mol]: 153.18
CAS: 1984-04-9

Physical Properties

Property code	Value	Unit	Source
gf	384.35	kJ/mol	Joback Method
hf	310.64	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	3.391		Crippen Method
mcvol	124.010	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	603.80	K	Joback Method
tc	855.02	K	Joback Method
tf	350.36	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.92	J/mol×K	603.80	Joback Method
cpg	286.01	J/mol×K	645.67	Joback Method
cpg	296.16	J/mol×K	687.54	Joback Method
cpg	305.46	J/mol×K	729.41	Joback Method
cpg	314.00	J/mol×K	771.28	Joback Method
cpg	321.87	J/mol×K	813.15	Joback Method
cpg	329.14	J/mol×K	855.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1984049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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