1-Naphthyl isocyanate

Other names:	Isocyanic acid, 1-naphthyl ester
	«alpha»-Naphthyl isocyanate
	1-Isocyanatonaphthalene
	1-Naphthyl isocyanate
Inchi:	InChI=1S/C11H7NO/c13-8-12-11-7-3-5-9-4-1-2-6-10(9)11/h1-7H
InchiKey:	BDQNKCYCTYYMAA-UHFFFAOYSA-N
Formula:	C11H7NO
SMILES:	O=C=Nc1cccc2ccccc12
Mol. weight [g/mol]:	169.18

Physical Properties

Property code	Value	Unit	Source
chs	-5355.50 ± 4.20	kJ/mol	NIST Webbook
hf	93.68	kJ/mol	Cheméo Relay (1.0)
hfs	26.00 ± 4.20	kJ/mol	NIST Webbook
hvap	65.76	kJ/mol	Cheméo Relay (1.0)
ie	7.98	eV	Cheméo Relay (1.0)
log10ws	-3.66		Cheméo Relay (1.0)
logp	2.807		Crippen Method
mcvol	129.880	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	541.25	K	Cheméo Relay (1.0)
tc	827.00	K	Cheméo Relay (1.0)
tf	317.81	K	Cheméo Relay (1.0)
vc	0.469	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86840&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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