

1-Chloroacetamidonaphthalene

Other names:	Acetamide, 2-chloro-N-1-naphthalenyl- Acetamide, 2-chloro-N-1-naphthyl- Chloroacetyl-1-naphthylamide 2-Chloro-N-(1-naphthyl)acetamide Acetamide, N-(1-naphthyl)-2-chloro-
Inchi:	InChI=1S/C12H10ClNO/c13-8-12(15)14-11-7-3-5-9-4-1-2-6-10(9)11/h1-7H,8H2,(H,14,15)
InchiKey:	CVRUANQADYCNLO-UHFFFAOYSA-N
Formula:	C12H10ClNO
SMILES:	O=C(CCl)Nc1cccc2ccccc12
Mol. weight [g/mol]:	219.67
CAS:	832-89-3

Physical Properties

Property code	Value	Unit	Source
gf	208.13	kJ/mol	Joback Method
hf	50.27	kJ/mol	Joback Method
hfus	28.40	kJ/mol	Joback Method
hvap	64.45	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.017		Crippen Method
mcvol	160.510	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	666.07	K	Joback Method
tc	905.71	K	Joback Method
tf	429.15	K	Joback Method
vc	0.612	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.80	J/mol×K	666.07	Joback Method
cpg	395.87	J/mol×K	706.01	Joback Method

cpg	406.97	J/mol×K	745.95	Joback Method
cpg	417.17	J/mol×K	785.89	Joback Method
cpg	426.57	J/mol×K	825.83	Joback Method
cpg	435.25	J/mol×K	865.77	Joback Method
cpg	443.29	J/mol×K	905.71	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=C832893&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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