

Acetamide, N-(1-naphthyl)-2,2-dichloro-

Inchi:	InChI=1S/C12H9Cl2NO/c13-11(14)12(16)15-10-7-3-5-8-4-1-2-6-9(8)10/h1-7,11H,(H,15,1
InchiKey:	SJVSQQFAACIPOJ-UHFFFAOYSA-N
Formula:	C12H9Cl2NO
SMILES:	O=C(Nc1cccc2ccccc12)C(Cl)Cl
Mol. weight [g/mol]:	254.11

Physical Properties

Property code	Value	Unit	Source
gf	193.76	kJ/mol	Joback Method
hf	29.25	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	68.45	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.582		Crippen Method
mcvol	172.750	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	2035.00		NIST Webbook
rinpol	2035.00		NIST Webbook
tb	703.06	K	Joback Method
tc	950.20	K	Joback Method
tf	444.07	K	Joback Method
vc	0.654	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.44	J/mol×K	703.06	Joback Method
cpg	417.61	J/mol×K	744.25	Joback Method
cpg	427.81	J/mol×K	785.44	Joback Method
cpg	437.13	J/mol×K	826.63	Joback Method
cpg	445.69	J/mol×K	867.82	Joback Method
cpg	453.57	J/mol×K	909.01	Joback Method
cpg	460.87	J/mol×K	950.20	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=U307305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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