

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

Inchi: InChI=1S/C12H8Cl3NO/c13-12(14,15)11(17)16-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,(H,16,17)
InchiKey: FEXNJZJFISBCHC-UHFFFAOYSA-N
Formula: C12H8Cl3NO
SMILES: O=C(Nc1cccc2ccccc12)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 288.56

Physical Properties

Property code	Value	Unit	Source
gf	187.11	kJ/mol	Joback Method
hf	10.04	kJ/mol	Joback Method
hfus	29.38	kJ/mol	Joback Method
hvap	71.92	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.149		Crippen Method
mvol	184.990	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
tb	737.70	K	Joback Method
tc	996.42	K	Joback Method
tf	491.41	K	Joback Method
vc	0.699	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.29	J/mol×K	737.70	Joback Method
cpg	439.26	J/mol×K	780.82	Joback Method
cpg	448.27	J/mol×K	823.94	Joback Method
cpg	456.46	J/mol×K	867.06	Joback Method
cpg	464.00	J/mol×K	910.18	Joback Method
cpg	471.04	J/mol×K	953.30	Joback Method
cpg	477.72	J/mol×K	996.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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