

2-Chloro-N,N-diethylacetamide

Other names:	Butanamide, 2-chloro-N,N-diethyl-3-oxo- 2-chloro-N,N-diethyl-3-oxobutyramide
Inchi:	InChI=1S/C8H14ClNO2/c1-4-10(5-2)8(12)7(9)6(3)11/h7H,4-5H2,1-3H3
InchiKey:	SEWWCLPPLUYJOT-UHFFFAOYSA-N
Formula:	C8H14ClNO2
SMILES:	CCN(CC)C(=O)C(Cl)C(C)=O
Mol. weight [g/mol]:	191.66
CAS:	15844-87-8

Physical Properties

Property code	Value	Unit	Source
gf	-144.95	kJ/mol	Joback Method
hf	-387.10	kJ/mol	Joback Method
hfus	23.37	kJ/mol	Joback Method
hvap	52.93	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.051		Crippen Method
mvol	148.940	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
tb	539.61	K	Joback Method
tc	732.23	K	Joback Method
tf	327.17	K	Joback Method
vc	0.556	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.54	J/molxK	539.61	Joback Method
cpg	347.77	J/molxK	571.71	Joback Method
cpg	359.35	J/molxK	603.82	Joback Method
cpg	370.29	J/molxK	635.92	Joback Method
cpg	380.63	J/molxK	668.02	Joback Method
cpg	390.37	J/molxK	700.12	Joback Method
cpg	399.54	J/molxK	732.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.50 ± 0.50	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15844878&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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