

Benzanilide, 2-(n-methyl-chloroacetamido)-

Inchi:	InChI=1S/C16H15ClN2O2/c1-19(15(20)11-17)14-10-6-5-9-13(14)16(21)18-12-7-3-2-4-8-
InchiKey:	HXLVSWGUYUKUEDT-UHFFFAOYSA-N
Formula:	C16H15ClN2O2
SMILES:	CN(C(=O)CCl)c1ccccc1C(=O)Nc1ccccc1
Mol. weight [g/mol]:	302.76
CAS:	1229-34-1

Physical Properties

Property code	Value	Unit	Source
gf	229.43	kJ/mol	Joback Method
hf	-31.88	kJ/mol	Joback Method
hfus	40.40	kJ/mol	Joback Method
hvap	82.78	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.140		Crippen Method
mcvol	224.120	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
tb	831.60	K	Joback Method
tc	1070.48	K	Joback Method
tf	550.35	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.94	J/molxK	831.60	Joback Method
cpg	633.24	J/molxK	871.41	Joback Method
cpg	644.45	J/molxK	911.23	Joback Method
cpg	654.64	J/molxK	951.04	Joback Method
cpg	663.91	J/molxK	990.85	Joback Method
cpg	672.36	J/molxK	1030.67	Joback Method
cpg	680.07	J/molxK	1070.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1229341&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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