

N-(2-CHLOROETHYL)BENZAMIDE

Other names:	Benzamide, N-(2-chloroethyl)-
Inchi:	InChI=1S/C9H10ClNO/c10-6-7-11-9(12)8-4-2-1-3-5-8/h1-5H,6-7H2,(H,11,12)
InchiKey:	FYQJUYCGPLFWQR-UHFFFAOYSA-N
Formula:	C9H10ClNO
SMILES:	O=C(NCCCl)c1ccccc1
Mol. weight [g/mol]:	183.64

Physical Properties

Property code	Value	Unit	Source
af	0.5454		Cheméo Relay (1.0)
gf	85.85	kJ/mol	Joback Method
hf	-152.59	kJ/mol	Cheméo Relay (1.0)
hfus	24.00	kJ/mol	Joback Method
hvap	74.84	kJ/mol	Cheméo Relay (1.0)
ie	9.45	eV	Cheméo Relay (1.0)
log10ws	-2.38		Cheméo Relay (1.0)
logp	1.655		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	563.26	K	Cheméo Relay (1.0)
tc	808.91	K	Cheméo Relay (1.0)
tf	320.95	K	Cheméo Relay (1.0)
vc	0.476	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.51	J/mol×K	573.47	Joback Method
cpg	315.62	J/mol×K	610.67	Joback Method
cpg	326.88	J/mol×K	647.87	Joback Method
cpg	337.34	J/mol×K	685.07	Joback Method
cpg	347.04	J/mol×K	722.27	Joback Method
cpg	356.01	J/mol×K	759.47	Joback Method
cpg	364.29	J/mol×K	796.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26385079&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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