Aklomide

Other names:	Benzamide, 2-chloro-4-nitro-
	Aklomix
	Alkomide
	2-Chloro-4-nitrobenzamide
	Clomide
	NSC 191832
Inchi:	InChI=1S/C7H5ClN2O3/c8-6-3-4(10(12)13)1-2-5(6)7(9)11/h1-3H,(H2,9,11)
InchiKey:	GFGSZUNNBQXGMK-UHFFFAOYSA-N
Formula:	C7H5ClN2O3
SMILES:	NC(=O)c1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]:	200.58
CAS:	3011-89-0

Physical Properties

Property code	Value	Unit	Source
gf	62.36	kJ/mol	Joback Method
hf	-79.51	kJ/mol	Joback Method
hfus	29.50	kJ/mol	Joback Method
hvap	73.14	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	1.347		Crippen Method
mcvol	126.940	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
tb	711.87	K	Joback Method
tc	978.24	K	Joback Method
tf	526.83	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.35	J/mol×K	711.87	Joback Method
cpg	303.50	J/mol×K	756.27	Joback Method
cpg	310.87	J/mol×K	800.66	Joback Method

cpg	317.49	J/mol×K	845.06	Joback Method
cpg	323.40	J/mol×K	889.45	Joback Method
cpg	328.66	J/mol×K	933.85	Joback Method
cpg	333.29	J/mol×K	978.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3011890&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume