

Benzoic acid, 3-amino-2,5-dichloro-

Other names:	2,5-Dichloro-3-aminobenzoic acid 3-Amino-2,5-dichlorobenzoic acid ACP-M-728 Acpm-629 Ambiben Amiben Amiben ds Amibin Amoben Chlorambed Chloramben Chlorambene Kyselina 3-amino-2,5-dichlorbenzoova NCI-C00055 Ornamental weeder Ornamental weeder 4G Vegaben Vegiben
Inchi:	InChI=1S/C7H5Cl2NO2/c8-3-1-4(7(11)12)6(9)5(10)2-3/h1-2H,10H2,(H,11,12)
InchiKey:	HSSBORCLYSCBJR-UHFFFAOYSA-N
Formula:	C7H5Cl2NO2
SMILES:	<chem>Nc1cc(Cl)cc(C(=O)O)c1Cl</chem>
Mol. weight [g/mol]:	206.03
CAS:	133-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-131.57	kJ/mol	Joback Method
hf	-248.19	kJ/mol	Joback Method
hfus	26.04	kJ/mol	Joback Method
hvap	78.27	kJ/mol	Joback Method
log10ws	-2.47		Aqueous Solubility Prediction Method
logp	2.274		Crippen Method
mcvol	127.630	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	694.62	K	Joback Method

tc	921.79	K	Joback Method
tf	475.75 ± 0.20	K	NIST Webbook
tf	474.50 ± 0.20	K	NIST Webbook
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.93	J/mol×K	694.62	Joback Method
cpg	280.35	J/mol×K	732.48	Joback Method
cpg	286.29	J/mol×K	770.34	Joback Method
cpg	291.76	J/mol×K	808.21	Joback Method
cpg	296.79	J/mol×K	846.07	Joback Method
cpg	301.40	J/mol×K	883.93	Joback Method
cpg	305.59	J/mol×K	921.79	Joback Method
hfust	37.42	kJ/mol	475.60	NIST Webbook
hfust	37.42	kJ/mol	475.60	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C133904&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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
hfust:	Enthalpy of fusion at a given temperature
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

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