3,5-Dibromoanthranilic acid

Other names:	2-Amino-3,5-dibromobenzoic acid
	Benzoic acid, 2-amino-3,5-dibromo-
Inchi:	InChI=1S/C7H5Br2NO2/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2H,10H2,(H,11,12)
InchiKey:	WNABMWFLKQEGCP-UHFFFAOYSA-N
Formula:	C7H5Br2NO2
SMILES:	Nc1c(Br)cc(Br)cc1C(=O)O
Mol. weight [g/mol]:	294.93
CAS:	609-85-8

Physical Properties

Property code	Value	Unit	Source
gf	-79.07	kJ/mol	Joback Method
hf	-164.05	kJ/mol	Joback Method
hfus	28.21	kJ/mol	Joback Method
hvap	82.37	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.492		Crippen Method
mcvol	138.150	ml/mol	McGowan Method
pc	6359.24	kPa	Joback Method
tb	752.08	K	Joback Method
tc	994.37	K	Joback Method
tf	505.15 ± 3.00	K	NIST Webbook
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.97	J/mol×K	752.08	Joback Method
cpg	290.83	J/mol×K	792.46	Joback Method
cpg	296.24	J/mol×K	832.84	Joback Method
cpg	301.23	J/mol×K	873.22	Joback Method
cpg	305.83	J/mol×K	913.61	Joback Method
cpg	310.11	J/mol×K	953.99	Joback Method
cpg	314.09	J/mol×K	994.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C609858&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