5-Bromoanthranalic acid

Other names:	2-amino-5-bromobenzoic acid
	5-Bromo-2-aminobenzoic acid
	5-Bromoanthranilic acid
	Anthranilic acid, 5-bromo-
	Benzoic acid, 2-amino-5-bromo-
Inchi:	InChI=1S/C7H6BrNO2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,9H2,(H,10,11)
InchiKey:	CUKXRHLWPSBCTI-UHFFFAOYSA-N
Formula:	C7H6BrNO2
SMILES:	Nc1ccc(Br)cc1C(=O)O
Mol. weight [g/mol]:	216.03

Physical Properties

Property code	Value	Unit	Source
hf	-286.07	kJ/mol	Cheméo Relay (1.0)
hfus	23.32	kJ/mol	Joback Method
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-3.07		Aqueous Solubility Prediction Method
logp	1.730		Crippen Method
mcvol	120.650	ml/mol	McGowan Method
tb	590.35	K	Cheméo Relay (1.0)
tf	493.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.54	J/mol×K	680.94	Joback Method
cpg	271.55	J/mol×K	719.50	Joback Method
cpg	278.02	J/mol×K	758.05	Joback Method
cpg	284.00	J/mol×K	796.61	Joback Method
cpg	289.52	J/mol×K	835.16	Joback Method
cpg	294.60	J/mol×K	873.72	Joback Method
cpg	299.27	J/mol×K	912.27	Joback Method

Sources

Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5794887&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
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point