azathioprine

Inchi: InChI=1S/C7H6BrNO2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,9H2,(H,10,11)
InchiKey: LMEKQMALGUDUQG-UHFFFAOYSA-N
Formula: C7H6BrNO2
SMILES: Nc1ccc(Br)cc1C(=O)O
Mol. weight [g/mol]: 216.03

Physical Properties

Property code	Value	Unit	Source
gf	-83.76	kJ/mol	Joback Method
hf	-178.91	kJ/mol	Joback Method
hfus	23.32	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-3.21		Aqueous Solubility Prediction Method
log10ws	-3.44		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.730		Crippen Method
mcvol	120.650	ml/mol	McGowan Method
pc	5845.00	kPa	Joback Method
tb	680.94	K	Joback Method
tc	912.27	K	Joback Method
tf	492.65	K	Aqueous Solubility Prediction Method
vc	0.435	m3/kmol	Joback Method

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

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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