C7H6Br3N

Inchi: InChI=1S/C7H6Br3N/c1-3-4(8)2-5(9)7(11)6(3)10/h2H,11H2,1H3
InchiKey: KDZKZKWJNMBNAP-UHFFFAOYSA-N
Formula: C7H6Br3N
SMILES: Cc1c(Br)cc(Br)c(N)c1Br
Mol. weight [g/mol]: 343.84
CAS: 71642-16-5

Physical Properties

Property code	Value	Unit	Source
gf	191.36	kJ/mol	Joback Method
hf	115.62	kJ/mol	Joback Method
hfus	27.42	kJ/mol	Joback Method
hvap	66.05	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.865		Crippen Method
mcvol	148.210	ml/mol	McGowan Method
pc	5446.55	kPa	Joback Method
tb	677.17	K	Joback Method
tc	951.74	K	Joback Method
tf	507.81	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.10	J/mol×K	677.17	Joback Method
cpg	277.58	J/mol×K	722.93	Joback Method
cpg	284.48	J/mol×K	768.69	Joback Method
cpg	290.88	J/mol×K	814.46	Joback Method
cpg	296.84	J/mol×K	860.22	Joback Method
cpg	302.42	J/mol×K	905.98	Joback Method
cpg	307.68	J/mol×K	951.74	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71642165&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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