6-Chloro-7-sulfamyl-3(4h)-oxo-1,2,4-benzothiadiaz

Inchi: InChI=1S/C7H6ClN3O5S2/c8-3-1-4-6(2-5(3)17(9,13)14)18(15,16)11-7(12)10-4/h1-2H,(H
InchiKey: CLWJBTNSDQIMNT-UHFFFAOYSA-N
Formula: C7H6ClN3O5S2
SMILES: NS(=O)(=O)c1cc2c(cc1Cl)NC(=O)NS2(=O)=O
Mol. weight [g/mol]: 311.72
CAS: 89813-56-9

Physical Properties

Property code	Value	Unit	Source
gf	-675.05	kJ/mol	Joback Method
hf	-846.05	kJ/mol	Joback Method
hfus	52.09	kJ/mol	Joback Method
hvap	104.89	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	-0.189		Crippen Method
mcvol	174.800	ml/mol	McGowan Method
pc	9536.74	kPa	Joback Method
tb	766.35	K	Joback Method
tc	1015.09	K	Joback Method
tf	768.92	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.65	J/mol×K	766.35	Joback Method
cpg	443.37	J/mol×K	807.81	Joback Method
cpg	451.87	J/mol×K	849.26	Joback Method
cpg	459.11	J/mol×K	890.72	Joback Method
cpg	465.02	J/mol×K	932.18	Joback Method
cpg	469.55	J/mol×K	973.64	Joback Method
cpg	472.65	J/mol×K	1015.09	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=C89813569&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