5,6-Dichloro-7-sulfamyl-3,4-dihydro-1,2,4-benzoth

Inchi: InChI=1S/C7H7Cl2N3O4S2/c8-5-3(17(10,13)14)1-4-7(6(5)9)11-2-12-18(4,15)16/h1,11-12
InchiKey: BSNKBIJVLZUERH-UHFFFAOYSA-N
Formula: C7H7Cl2N3O4S2
SMILES: NS(=O)(=O)c1cc2c(c(Cl)c1Cl)NCNS2(=O)=O
Mol. weight [g/mol]: 332.18
CAS: 5233-42-1

Physical Properties

Property code	Value	Unit	Source
gf	-574.02	kJ/mol	Joback Method
hf	-735.56	kJ/mol	Joback Method
hfus	56.39	kJ/mol	Joback Method
hvap	105.69	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	0.302		Crippen Method
mcvol	185.470	ml/mol	McGowan Method
pc	8101.62	kPa	Joback Method
tb	740.94	K	Joback Method
tc	982.61	K	Joback Method
tf	743.14	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.67	J/mol×K	740.94	Joback Method
cpg	444.19	J/mol×K	781.22	Joback Method
cpg	452.68	J/mol×K	821.50	Joback Method
cpg	460.15	J/mol×K	861.77	Joback Method
cpg	466.58	J/mol×K	902.05	Joback Method
cpg	471.95	J/mol×K	942.33	Joback Method
cpg	476.26	J/mol×K	982.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5233421&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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