3-[(Dichloroamino)sulfonyl]benzoic acid

Inchi: InChI=1S/C7H5Cl2NO4S/c8-10(9)15(13,14)6-3-1-2-5(4-6)7(11)12/h1-4H,(H,11,12)
InchiKey: JVIMBTOZWCVXRU-UHFFFAOYSA-N
Formula: C7H5Cl2NO4S
SMILES: O=C(O)c1cccc(S(=O)(=O)N(Cl)Cl)c1
Mol. weight [g/mol]: 270.09
CAS: 116465-30-6

Physical Properties

Property code	Value	Unit	Source
gf	-536.52	kJ/mol	Joback Method
hf	-644.86	kJ/mol	Joback Method
hfus	36.02	kJ/mol	Joback Method
hvap	86.99	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.683		Crippen Method
mcvol	155.720	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
tb	672.35	K	Joback Method
tc	880.47	K	Joback Method
tf	449.21	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.38	J/mol×K	672.35	Joback Method
cpg	351.04	J/mol×K	707.04	Joback Method
cpg	358.03	J/mol×K	741.72	Joback Method
cpg	364.35	J/mol×K	776.41	Joback Method
cpg	370.04	J/mol×K	811.09	Joback Method
cpg	375.09	J/mol×K	845.78	Joback Method
cpg	379.53	J/mol×K	880.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116465306&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