4-Chloro-6-aminobenzene-1,3-disulfonyl chloride

Other names: 4-amino-6-chlorobenzene-1,3-di(sulphonyl chloride)
Inchi: InChI=1S/C6H4Cl3NO4S2/c7-3-1-4(10)6(16(9,13)14)2-5(3)15(8,11)12/h1-2H,10H2
InchiKey: YIZXGHNDQUYDDF-UHFFFAOYSA-N
Formula: C6H4Cl3NO4S2
SMILES: Nc1cc(Cl)c(S(=O)(=O)Cl)cc1S(=O)(=O)Cl
Mol. weight [g/mol]: 324.59
CAS: 671-89-6

Physical Properties

Property code	Value	Unit	Source
gf	-823.26	kJ/mol	Joback Method
hf	-885.18	kJ/mol	Joback Method
hfus	44.71	kJ/mol	Joback Method
hvap	94.28	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	1.777		Crippen Method
mcvol	174.520	ml/mol	McGowan Method
pc	6379.57	kPa	Joback Method
tb	658.68	K	Joback Method
tc	886.79	K	Joback Method
tf	471.50	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.79	J/mol×K	658.68	Joback Method
cpg	364.98	J/mol×K	696.70	Joback Method
cpg	372.40	J/mol×K	734.72	Joback Method
cpg	379.02	J/mol×K	772.74	Joback Method
cpg	384.81	J/mol×K	810.75	Joback Method
cpg	389.75	J/mol×K	848.77	Joback Method
cpg	393.81	J/mol×K	886.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C671896&Units=SI

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