2-Cyanobenzenesulfonyl chloride

Inchi: InChI=1S/C7H4ClNO2S/c8-12(10,11)7-4-2-1-3-6(7)5-9/h1-4H
InchiKey: NQAYCMBZPAARNO-UHFFFAOYSA-N
Formula: C7H4ClNO2S
SMILES: N#Cc1ccccc1S(=O)(=O)Cl
Mol. weight [g/mol]: 201.63
CAS: 69360-26-5

Physical Properties

Property code	Value	Unit	Source
gf	-236.45	kJ/mol	Joback Method
hf	-266.96	kJ/mol	Joback Method
hfus	24.62	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.486		Crippen Method
mcvol	127.440	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	578.51	K	Joback Method
tc	810.14	K	Joback Method
tf	341.06	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.92	J/mol×K	578.51	Joback Method
cpg	261.64	J/mol×K	617.12	Joback Method
cpg	269.69	J/mol×K	655.72	Joback Method
cpg	277.09	J/mol×K	694.33	Joback Method
cpg	283.83	J/mol×K	732.93	Joback Method
cpg	289.92	J/mol×K	771.54	Joback Method
cpg	295.36	J/mol×K	810.14	Joback Method

Sources

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=C69360265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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