Pentafluorobenzenesulfonyl chloride

Other names:	Benzenesulfonyl chloride, pentafluoro- Pentafluorophenylsulfonyl chloride 2,3,4,5,6-Pentafluoro-benzenesulfonyl chloride Benzene,1-chlorosulphonyl-2,3,4,5,6-pentafluoro- pentafluorobenzenesulphonyl chloride
Inchi:	InChI=1S/C6ClF5O2S/c7-15(13,14)6-4(11)2(9)1(8)3(10)5(6)12
InchiKey:	UOJCTEGNHXRPKO-UHFFFAOYSA-N
Formula:	C6ClF5O2S
SMILES:	O=S(=O)(Cl)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	266.57
CAS:	832-53-1

Physical Properties

Property code	Value	Unit	Source
gf	-1390.62	kJ/mol	Joback Method
hf	-1437.63	kJ/mol	Joback Method
hfus	34.37	kJ/mol	Joback Method
hvap	53.47	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.310		Crippen Method
mcvol	120.820	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
tb	483.50 ± 0.50	K	NIST Webbook
tc	641.31	K	Joback Method
tf	317.83	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.49	J/mol×K	469.82	Joback Method
cpg	242.69	J/mol×K	498.40	Joback Method
cpg	248.67	J/mol×K	526.98	Joback Method
cpg	254.42	J/mol×K	555.57	Joback Method

cpg	259.94	J/mol×K	584.15	Joback Method
cpg	265.22	J/mol×K	612.73	Joback Method
cpg	270.24	J/mol×K	641.31	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=C832531&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