3,5-Bis(trifluoromethyl)benzenesulfonyl chloride

Other names: 3,5-Di(trifluoromethyl)benzene sulfonyl chloride
Benzenesulfonyl chloride, 3,5-bis(trifluoromethyl)-
3,5-bis(trifluoromethyl)benzenesulphonyl chloride

Inchi: InChI=1S/C8H3ClF6O2S/c9-18(16,17)6-2-4(7(10,11)12)1-5(3-6)8(13,14)15/h1-3H

InchiKey: BTRCVKADYDVSLI-UHFFFAOYSA-N

Formula: C8H3ClF6O2S

SMILES: O=S(=O)(Cl)c1cc(C(F)(F)F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 312.62

CAS: 39234-86-1

Physical Properties

Property code	Value	Unit	Source
gf	-1534.02	kJ/mol	Joback Method
hf	-1658.11	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	52.53	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.652		Crippen Method
mcvol	150.770	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
tb	493.45	K	Joback Method
tc	670.31	K	Joback Method
tf	308.24	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.54	J/mol×K	493.45	Joback Method
cpg	342.96	J/mol×K	522.93	Joback Method
cpg	352.65	J/mol×K	552.40	Joback Method
cpg	361.65	J/mol×K	581.88	Joback Method
cpg	369.98	J/mol×K	611.36	Joback Method
cpg	377.66	J/mol×K	640.83	Joback Method

cpg	384.73	J/mol×K	670.31	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=C39234861&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