3,4,5-Tris(methylthio)benzotrifluoride

Inchi: InChI=1S/C10H11F3S3/c1-14-7-4-6(10(11,12)13)5-8(15-2)9(7)16-3/h4-5H,1-3H3
InchiKey: FQGDLFLKJDPASE-UHFFFAOYSA-N
Formula: C10H11F3S3
SMILES: CSc1cc(C(F)(F)F)cc(SC)c1SC
Mol. weight [g/mol]: 284.38
CAS: 65516-85-0

Physical Properties

Property code	Value	Unit	Source
gf	-365.39	kJ/mol	Joback Method
hf	-519.08	kJ/mol	Joback Method
hfus	28.75	kJ/mol	Joback Method
hvap	58.82	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.871		Crippen Method
mcvol	182.360	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
tb	670.74	K	Joback Method
tc	916.08	K	Joback Method
tf	373.83	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.07	J/mol×K	670.74	Joback Method
cpg	448.76	J/mol×K	711.63	Joback Method
cpg	460.40	J/mol×K	752.52	Joback Method
cpg	471.02	J/mol×K	793.41	Joback Method
cpg	480.65	J/mol×K	834.30	Joback Method
cpg	489.31	J/mol×K	875.19	Joback Method
cpg	497.03	J/mol×K	916.08	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=C65516850&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