Ethyl trifluoromethyl disulfide

Inchi: InChI=1S/C3H5F3S2/c1-2-7-8-3(4,5)6/h2H2,1H3
InchiKey: MTLRRZISTVKFFN-UHFFFAOYSA-N
Formula: C3H5F3S2
SMILES: CCSSC(F)(F)F
Mol. weight [g/mol]: 162.20
CAS: 691-05-4

Physical Properties

Property code	Value	Unit	Source
gf	-540.97	kJ/mol	Joback Method
hf	-618.59	kJ/mol	Joback Method
hfus	13.61	kJ/mol	Joback Method
hvap	32.16	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.907		Crippen Method
mcvol	91.140	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	400.18	K	Joback Method
tc	599.03	K	Joback Method
tf	196.56	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.32	J/mol×K	565.89	Joback Method
cpg	167.64	J/mol×K	400.18	Joback Method
cpg	175.45	J/mol×K	433.32	Joback Method
cpg	182.81	J/mol×K	466.46	Joback Method
cpg	189.73	J/mol×K	499.61	Joback Method
cpg	196.23	J/mol×K	532.75	Joback Method
cpg	208.01	J/mol×K	599.03	Joback Method
hvapt	33.80	kJ/mol	278.00	NIST Webbook

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=C691054&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
hvapt:	Enthalpy of vaporization at a given temperature
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