CF3CH2SC2H5

Inchi: InChI=1S/C4H7F3S/c1-2-8-3-4(5,6)7/h2-3H2,1H3
InchiKey: HGTCKYWIBWROKM-UHFFFAOYSA-N
Formula: C4H7F3S
SMILES: CCSCC(F)(F)F
Mol. weight [g/mol]: 144.16
CAS: 5187-62-2

Physical Properties

Property code	Value	Unit	Source
affp	797.60	kJ/mol	NIST Webbook
basg	766.40	kJ/mol	NIST Webbook
gf	-565.67	kJ/mol	Joback Method
hf	-681.10	kJ/mol	Joback Method
hfus	12.07	kJ/mol	Joback Method
hvap	27.57	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.302		Crippen Method
mcvol	88.880	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	354.28	K	Joback Method
tc	526.11	K	Joback Method
tf	173.43	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.07	J/mol×K	354.28	Joback Method
cpg	169.75	J/mol×K	382.92	Joback Method
cpg	178.00	J/mol×K	411.56	Joback Method
cpg	185.83	J/mol×K	440.20	Joback Method
cpg	193.25	J/mol×K	468.83	Joback Method
cpg	200.29	J/mol×K	497.47	Joback Method
cpg	206.95	J/mol×K	526.11	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=C5187622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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