CF3COSCH3

Inchi: InChI=1S/C3H3F3OS/c1-8-2(7)3(4,5)6/h1H3
InchiKey: JOURTNKOBNXXIV-UHFFFAOYSA-N
Formula: C3H3F3OS
SMILES: CSC(=O)C(F)(F)F
Mol. weight [g/mol]: 144.12
CAS: 41879-94-1

Physical Properties

Property code	Value	Unit	Source
affp	765.20	kJ/mol	NIST Webbook
basg	734.30	kJ/mol	NIST Webbook
gf	-703.01	kJ/mol	Joback Method
hf	-773.04	kJ/mol	Joback Method
hfus	11.08	kJ/mol	Joback Method
hvap	32.09	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	1.438		Crippen Method
mcvol	76.360	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	385.27	K	Joback Method
tc	572.00	K	Joback Method
tf	212.09	K	Joback Method
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.98	J/mol×K	385.27	Joback Method
cpg	147.56	J/mol×K	416.39	Joback Method
cpg	153.75	J/mol×K	447.51	Joback Method
cpg	159.55	J/mol×K	478.64	Joback Method
cpg	164.98	J/mol×K	509.76	Joback Method
cpg	170.06	J/mol×K	540.88	Joback Method
cpg	174.79	J/mol×K	572.00	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=C41879941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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