C2HF3OS

Inchi: InChI=1S/C2HF3OS/c3-2(4,5)1(6)7/h(H,6,7)
InchiKey: HLDPDUFAJCWOBX-UHFFFAOYSA-N
Formula: C2HF3OS
SMILES: OC(=S)C(F)(F)F
Mol. weight [g/mol]: 130.09
CAS: 2925-25-9

Physical Properties

Property code	Value	Unit	Source
gf	-635.39	kJ/mol	Joback Method
hf	-687.42	kJ/mol	Joback Method
hfus	11.45	kJ/mol	Joback Method
hvap	39.71	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.434		Crippen Method
mcvol	62.270	ml/mol	McGowan Method
pc	5552.58	kPa	Joback Method
tb	401.96	K	Joback Method
tc	575.94	K	Joback Method
tf	211.58	K	Joback Method
vc	0.245	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.72	J/mol×K	401.96	Joback Method
cpg	122.17	J/mol×K	430.96	Joback Method
cpg	126.17	J/mol×K	459.95	Joback Method
cpg	129.75	J/mol×K	488.95	Joback Method
cpg	132.95	J/mol×K	517.95	Joback Method
cpg	135.80	J/mol×K	546.94	Joback Method
cpg	138.32	J/mol×K	575.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2925259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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