CH2F3NO2S

Inchi: InChI=1S/CH2F3NO2S/c2-1(3,4)8(5,6)7/h(H2,5,6,7)
InchiKey: KAKQVSNHTBLJCH-UHFFFAOYSA-N
Formula: CH2F3NO2S
SMILES: NS(=O)(=O)C(F)(F)F
Mol. weight [g/mol]: 149.09
CAS: 421-85-2

Physical Properties

Property code	Value	Unit	Source
gf	-1026.14	kJ/mol	Joback Method
hf	-1080.61	kJ/mol	Joback Method
hfus	16.75	kJ/mol	Joback Method
hvap	43.35	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	-0.205		Crippen Method
mcvol	68.330	ml/mol	McGowan Method
pc	6740.71	kPa	Joback Method
tb	337.17	K	Joback Method
tc	500.14	K	Joback Method
tf	227.04	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.72	J/mol×K	337.17	Joback Method
cpg	136.38	J/mol×K	364.33	Joback Method
cpg	141.75	J/mol×K	391.49	Joback Method
cpg	146.86	J/mol×K	418.66	Joback Method
cpg	151.70	J/mol×K	445.82	Joback Method
cpg	156.27	J/mol×K	472.98	Joback Method
cpg	160.58	J/mol×K	500.14	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C421852&Units=SI

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