Trifluoromethyl peroxynitrate

Inchi: InChI=1S/CF3NO4/c2-1(3,4)8-9-5(6)7
InchiKey: IRCOOTKZKSUTLW-UHFFFAOYSA-N
Formula: CF3NO4
SMILES: O=[N+]([O-])OOC(F)(F)F
Mol. weight [g/mol]: 147.01
CAS: 50311-48-3

Physical Properties

Property code	Value	Unit	Source
gf	-798.50	kJ/mol	Joback Method
hf	-936.25	kJ/mol	Joback Method
hfus	13.91	kJ/mol	Joback Method
hvap	35.48	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	0.646		Crippen Method
mcvol	59.420	ml/mol	McGowan Method
pc	4743.15	kPa	Joback Method
tb	413.54	K	Joback Method
tc	605.09	K	Joback Method
tf	293.29	K	Joback Method
vc	0.253	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.11	J/mol×K	413.54	Joback Method
cpg	134.58	J/mol×K	445.47	Joback Method
cpg	138.83	J/mol×K	477.39	Joback Method
cpg	142.85	J/mol×K	509.32	Joback Method
cpg	146.66	J/mol×K	541.24	Joback Method
cpg	150.24	J/mol×K	573.17	Joback Method
cpg	153.60	J/mol×K	605.09	Joback Method
hvapt	24.80	kJ/mol	220.00	NIST Webbook

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=C50311483&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
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