1-Fluoro-1,1-dinitroethane

Inchi: InChI=1S/C2H3FN2O4/c1-2(3,4(6)7)5(8)9/h1H3
InchiKey: INUKSLQNFYBSOB-UHFFFAOYSA-N
Formula: C2H3FN2O4
SMILES: CC(F)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 138.05
CAS: 13214-58-9

Physical Properties

Property code	Value	Unit	Source
gf	-154.91	kJ/mol	Joback Method
hf	-256.00	kJ/mol	NIST Webbook
hfl	-303.00	kJ/mol	NIST Webbook
hfus	19.32	kJ/mol	Joback Method
hvap	46.40	kJ/mol	NIST Webbook
log10ws	-1.78		Crippen Method
logp	0.183		Crippen Method
mcvol	75.650	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
tb	544.88	K	Joback Method
tc	795.57	K	Joback Method
tf	402.53	K	Joback Method
vc	0.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.85	J/mol×K	544.88	Joback Method
cpg	182.88	J/mol×K	586.66	Joback Method
cpg	189.20	J/mol×K	628.44	Joback Method
cpg	194.87	J/mol×K	670.23	Joback Method
cpg	199.96	J/mol×K	712.01	Joback Method
cpg	204.51	J/mol×K	753.79	Joback Method
cpg	208.58	J/mol×K	795.57	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=C13214589&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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