1,1,2-Trifluorotrinitroethane

Inchi: InChI=1S/C2F3N3O6/c3-1(4,6(9)10)2(5,7(11)12)8(13)14
InchiKey: YZXMNZPACCLUCJ-UHFFFAOYSA-N
Formula: C2F3N3O6
SMILES: O=[N+]([O-])C(F)(F)C(F)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 219.03
CAS: 20165-38-2

Physical Properties

Property code	Value	Unit	Source
chl	-648.00 ± 2.00	kJ/mol	NIST Webbook
gf	-506.14	kJ/mol	Joback Method
hf	-601.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-659.00 ± 3.00	kJ/mol	NIST Webbook
hfus	29.43	kJ/mol	Joback Method
hvap	57.70 ± 0.80	kJ/mol	NIST Webbook
log10ws	-2.68		Crippen Method
logp	0.033		Crippen Method
mcvol	96.610	ml/mol	McGowan Method
pc	4621.41	kPa	Joback Method
tb	692.03	K	Joback Method
tc	955.89	K	Joback Method
tf	549.74	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.51	J/mol×K	692.03	Joback Method
cpg	266.63	J/mol×K	736.01	Joback Method
cpg	270.99	J/mol×K	779.98	Joback Method
cpg	274.69	J/mol×K	823.96	Joback Method
cpg	277.86	J/mol×K	867.94	Joback Method
cpg	280.61	J/mol×K	911.91	Joback Method
cpg	283.06	J/mol×K	955.89	Joback Method

hvapt	57.70	kJ/mol	333.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20165382&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
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
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