1,2-Difluorotetranitroethane

Inchi: InChI=1S/C2F2N4O8/c3-1(5(9)10,6(11)12)2(4,7(13)14)8(15)16
InchiKey: BDYYJOSEHYEBKF-UHFFFAOYSA-N
Formula: C2F2N4O8
SMILES: O=[N+]([O-])C(F)([N+](=O)[O-])C(F)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 246.04
CAS: 20165-39-3

Physical Properties

Property code	Value	Unit	Source
chl	-730.00 ± 3.00	kJ/mol	NIST Webbook
gf	-275.78	kJ/mol	Joback Method
hf	-352.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-415.00 ± 4.20	kJ/mol	NIST Webbook
hfus	37.71	kJ/mol	Joback Method
hvap	62.80 ± 0.80	kJ/mol	NIST Webbook
log10ws	-2.91		Crippen Method
logp	-0.660		Crippen Method
mcvol	112.260	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
tb	844.60	K	Joback Method
tc	1137.10	K	Joback Method
tf	692.76	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.92	J/mol×K	844.60	Joback Method
cpg	317.76	J/mol×K	893.35	Joback Method
cpg	321.06	J/mol×K	942.10	Joback Method
cpg	323.99	J/mol×K	990.85	Joback Method
cpg	326.72	J/mol×K	1039.60	Joback Method
cpg	329.43	J/mol×K	1088.35	Joback Method
cpg	332.29	J/mol×K	1137.10	Joback Method

hvapt	62.80	kJ/mol	310.00	NIST Webbook

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=C20165393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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