

Ethane, 1,1,2,2-tetrafluoro-1,2-dinitro-

Inchi: InChI=1S/C2F4N2O4/c3-1(4,7(9)10)2(5,6)8(11)12
InchiKey: NELYAMNMZQGGAJ-UHFFFAOYSA-N
Formula: C2F4N2O4
SMILES: O=[N+]([O-])C(F)(F)C(F)(F)[N+](=O)[O-]
Mol. weight [g/mol]: 192.03
CAS: 356-16-1

Physical Properties

Property code	Value	Unit	Source
chl	-602.00 ± 2.00	kJ/mol	NIST Webbook
gf	-736.50	kJ/mol	Joback Method
hf	-812.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-880.00 ± 3.00	kJ/mol	NIST Webbook
hfus	21.15	kJ/mol	Joback Method
hvap	67.80 ± 0.80	kJ/mol	NIST Webbook
log10ws	-2.45		Crippen Method
logp	0.725		Crippen Method
mcvol	80.960	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
tb	331.70	K	NIST Webbook
tc	767.33	K	Joback Method
tf	406.72	K	Joback Method
vc	0.361	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.43	J/mol×K	691.37	Joback Method
cpg	230.12	J/mol×K	729.35	Joback Method
cpg	205.24	J/mol×K	539.46	Joback Method
cpg	211.65	J/mol×K	577.44	Joback Method
cpg	217.27	J/mol×K	615.42	Joback Method
cpg	222.17	J/mol×K	653.40	Joback Method
cpg	233.31	J/mol×K	767.33	Joback Method

hvapt	34.70	kJ/mol	296.00	NIST Webbook
hvapt	67.80	kJ/mol	323.00	NIST Webbook

Sources

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=C356161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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