Methane,(2-fluoro-2,2-dinitroethoxy)(2,2,2-trinitroe

Inchi: InChI=1S/C5H6FN5O12/c6-4(7(12)13,8(14)15)1-22-3-23-2-5(9(16)17,10(18)19)11(20)21
InchiKey: AEKWETJEQDKAET-UHFFFAOYSA-N
Formula: C5H6FN5O12
SMILES: O=[N+]([O-])C(F)(COCOCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 347.13
CAS: 30893-52-8

Physical Properties

Property code	Value	Unit	Source
chl	-2419.10 ± 2.90	kJ/mol	NIST Webbook
gf	-230.16	kJ/mol	Joback Method
hf	-678.38	kJ/mol	Joback Method
hfl	-642.00 ± 13.00	kJ/mol	NIST Webbook
hfus	56.14	kJ/mol	Joback Method
hvap	111.09	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	-1.362		Crippen Method
mcvol	181.920	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
tb	1110.65	K	Joback Method
tc	1397.84	K	Joback Method
tf	914.05	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.04	J/mol×K	1110.65	Joback Method
cpg	569.36	J/mol×K	1158.52	Joback Method
cpg	572.10	J/mol×K	1206.38	Joback Method
cpg	574.37	J/mol×K	1254.25	Joback Method
cpg	576.30	J/mol×K	1302.11	Joback Method
cpg	578.02	J/mol×K	1349.98	Joback Method
cpg	579.64	J/mol×K	1397.84	Joback Method

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=C30893528&Units=SI

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
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