Fluoropentanitroethane

Inchi: InChI=1S/C2FN5O10/c3-1(4(9)10,5(11)12)2(6(13)14,7(15)16)8(17)18
InchiKey: QXCMLBSYQBLNDK-UHFFFAOYSA-N
Formula: C2FN5O10
SMILES: O=[N+]([O-])C(F)([N+](=O)[O-])C([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 273.05
CAS: 23072-51-7

Physical Properties

Property code	Value	Unit	Source
chs	-810.90 ± 5.90	kJ/mol	NIST Webbook
gf	-45.42	kJ/mol	Joback Method
hf	-86.20 ± 8.40	kJ/mol	NIST Webbook
hfs	-155.00 ± 8.40	kJ/mol	NIST Webbook
hfus	45.99	kJ/mol	Joback Method
hsub	69.00	kJ/mol	NIST Webbook
hvap	99.59	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	-1.353		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
pc	5430.51	kPa	Joback Method
tb	997.17	K	Joback Method
tc	1313.02	K	Joback Method
tf	835.78	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.49	J/mol×K	997.17	Joback Method
cpg	366.71	J/mol×K	1049.81	Joback Method
cpg	369.84	J/mol×K	1102.45	Joback Method
cpg	373.12	J/mol×K	1155.10	Joback Method
cpg	376.77	J/mol×K	1207.74	Joback Method
cpg	381.02	J/mol×K	1260.38	Joback Method

cpg	386.10	J/mol×K	1313.02	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=C23072517&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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

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