

1-Fluoro-1,1,3,5,5-pentanitro-3-azaheptane

Inchi:	InChI=1S/C6H9FN6O10/c1-2-5(9(14)15,10(16)17)3-8(13(22)23)4-6(7,11(18)19)12(20)21
InchiKey:	HBVFVNPIJPIFCH-UHFFFAOYSA-N
Formula:	C6H9FN6O10
SMILES:	CCC(CN(CC(F)([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	344.17
CAS:	60569-14-4

Physical Properties

Property code	Value	Unit	Source
chs	-3423.00 ± 3.00	kJ/mol	NIST Webbook
gf	99.04	kJ/mol	Joback Method
hf	-367.05	kJ/mol	Joback Method
hfs	-403.30 ± 3.40	kJ/mol	NIST Webbook
hfus	59.37	kJ/mol	Joback Method
hvap	110.54	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	-0.683		Crippen Method
mcvol	194.250	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	1101.13	K	Joback Method
tc	1387.23	K	Joback Method
tf	913.33	K	Joback Method
vc	0.795	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.43	J/mol×K	1101.13	Joback Method
cpg	630.38	J/mol×K	1148.81	Joback Method
cpg	637.44	J/mol×K	1196.50	Joback Method
cpg	644.84	J/mol×K	1244.18	Joback Method
cpg	652.80	J/mol×K	1291.86	Joback Method
cpg	661.56	J/mol×K	1339.54	Joback Method
cpg	671.32	J/mol×K	1387.23	Joback Method

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=C60569144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
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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