1,7-Difluoro-1,1,3,5,7,7-hexanitro-3,5-diazaheptane

Inchi: InChI=1S/C5H6F2N8O12/c6-4(10(16)17,11(18)19)1-8(14(24)25)3-9(15(26)27)2-5(7,12(2
InchiKey: SGOLSSPCBCZHEA-UHFFFAOYSA-N
Formula: C5H6F2N8O12
SMILES: O=[N+]([O-])N(CN(CC(F)([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])CC(F)([N+](=O)[O-])[N+
Mol. weight [g/mol]: 408.14
CAS: 80308-93-6

Physical Properties

Property code	Value	Unit	Source
gf	42.14	kJ/mol	Joback Method
hf	-485.75	kJ/mol	Joback Method
hfus	74.25	kJ/mol	Joback Method
hvap	126.13	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	-1.715		Crippen Method
mcvol	209.330	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	1241.80	K	Joback Method
tc	1537.01	K	Joback Method
tf	1078.73	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.69	J/mol×K	1241.80	Joback Method
cpg	689.76	J/mol×K	1291.00	Joback Method
cpg	698.88	J/mol×K	1340.20	Joback Method
cpg	709.34	J/mol×K	1389.40	Joback Method
cpg	721.41	J/mol×K	1438.61	Joback Method
cpg	735.38	J/mol×K	1487.81	Joback Method
cpg	751.54	J/mol×K	1537.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80308936&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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