

1,7-Difluoro-1,1,5,7,7-pentanitro-5-aza-3-oxahepta

Inchi:	InChI=1S/C5H6F2N6O11/c6-4(9(14)15,10(16)17)1-8(13(22)23)3-24-2-5(7,11(18)19)12(20)
InchiKey:	SOLZWBGEHVEJDE-UHFFFAOYSA-N
Formula:	C5H6F2N6O11
SMILES:	O=[N+]([O-])N(COCC(F)([N+](=O)[O-])[N+](=O)[O-])CC(F)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	364.13
CAS:	80308-82-3

Physical Properties

Property code	Value	Unit	Source
chs	-2520.00 ± 4.60	kJ/mol	NIST Webbook
gf	-209.19	kJ/mol	Joback Method
hf	-674.74	kJ/mol	Joback Method
hfs	-664.00 ± 4.60	kJ/mol	NIST Webbook
hfus	61.05	kJ/mol	Joback Method
hvap	109.91	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	-1.192		Crippen Method
mcvol	187.800	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	1099.94	K	Joback Method
tc	1378.78	K	Joback Method
tf	924.88	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.67	J/molxK	1099.94	Joback Method
cpg	598.44	J/molxK	1146.41	Joback Method
cpg	603.04	J/molxK	1192.89	Joback Method
cpg	607.65	J/molxK	1239.36	Joback Method
cpg	612.44	J/molxK	1285.83	Joback Method
cpg	617.58	J/molxK	1332.31	Joback Method
cpg	623.23	J/molxK	1378.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80308823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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