

1,1,4,4-Tetrakis(difluoroamino)cyclohexane

Inchi:	InChI=1S/C6H8F8N4/c7-15(8)5(16(9)10)1-2-6(4-3-5,17(11)12)18(13)14/h1-4H2
InchiKey:	TWGYTNIQXDMHMV-UHFFFAOYSA-N
Formula:	C6H8F8N4
SMILES:	FN(F)C1(N(F)F)CCC(N(F)F)(N(F)F)CC1
Mol. weight [g/mol]:	288.14
CAS:	18273-26-2

Physical Properties

Property code	Value	Unit	Source
gf	-1109.96	kJ/mol	Joback Method
hf	-1401.47	kJ/mol	Joback Method
hfus	28.33	kJ/mol	Joback Method
hvap	28.40	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.237		Crippen Method
mcvol	138.620	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	395.96	K	Joback Method
tc	535.31	K	Joback Method
tf	342.92	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.59	J/molxK	395.96	Joback Method
cpg	330.64	J/molxK	419.18	Joback Method
cpg	344.68	J/molxK	442.41	Joback Method
cpg	357.79	J/molxK	465.63	Joback Method
cpg	370.02	J/molxK	488.86	Joback Method
cpg	381.44	J/molxK	512.08	Joback Method
cpg	392.11	J/molxK	535.31	Joback Method
hfust	46.02	kJ/mol	382.20	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C18273262&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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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