

[(nitroimino)bis[methylene(nitroimino)]]dimethyl diacetate

Other names:	1,7-Diacetoxy-2,4,6-trinitro-2,4,6-triazaheptane
Inchi:	InChI=1S/C8H14N6O10/c1-7(15)23-5-10(13(19)20)3-9(12(17)18)4-11(14(21)22)6-24-8(2)
InchiKey:	CHBKPOAEXQUKHL-UHFFFAOYSA-N
Formula:	C8H14N6O10
SMILES:	CC(=O)OCN(CN(CN(COC(C)=O)[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	354.23
CAS:	14173-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-12.37	kJ/mol	Joback Method
hf	-527.74	kJ/mol	Joback Method
hfus	65.20	kJ/mol	Joback Method
hvap	107.62	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	-1.576		Crippen Method
mcvol	220.660	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
tb	1027.86	K	Joback Method
tc	1270.24	K	Joback Method
tf	422.50 ± 0.50	K	NIST Webbook
vc	0.832	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.77	J/mol×K	1027.86	Joback Method
cpg	710.95	J/mol×K	1068.26	Joback Method
cpg	716.11	J/mol×K	1108.65	Joback Method
cpg	720.29	J/mol×K	1149.05	Joback Method
cpg	723.54	J/mol×K	1189.45	Joback Method
cpg	725.92	J/mol×K	1229.84	Joback Method
cpg	727.47	J/mol×K	1270.24	Joback Method
hfust	38.49	kJ/mol	422.50	NIST Webbook

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=C14173627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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