

Tetrakis(2,2,2-trinitroethyl(orthocarbonate

Inchi:	InChI=1S/C9H8N12O28/c22-10(23)5(11(24)25,12(26)27)1-46-9(47-2-6(13(28)29,14(30)31)32)33
InchiKey:	JPTHXHQVODRICI-UHFFFAOYSA-N
Formula:	C9H8N12O28
SMILES:	O=[N+](O-)]C(COC(OCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])(OCC([N+](=O)[O-])([N+](=O)[O-])
Mol. weight [g/mol]:	732.22
CAS:	14548-58-4

Physical Properties

Property code	Value	Unit	Source
chs	-3918.00 ± 4.20	kJ/mol	NIST Webbook
gf	45.70	kJ/mol	Joback Method
hf	-930.84	kJ/mol	Joback Method
hfs	-766.90 ± 4.20	kJ/mol	NIST Webbook
hfus	123.08	kJ/mol	Joback Method
hsub	179.00	kJ/mol	NIST Webbook
hvap	237.88	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	-4.400		Crippen Method
mcvol	370.190	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	2300.93	K	Joback Method
tc	2991.35	K	Joback Method
tf	2015.53	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1752.99	J/mol×K	2300.93	Joback Method
cpg	1953.54	J/mol×K	2416.00	Joback Method
cpg	2196.79	J/mol×K	2531.07	Joback Method
cpg	2487.08	J/mol×K	2646.14	Joback Method
cpg	2828.73	J/mol×K	2761.21	Joback Method
cpg	3226.08	J/mol×K	2876.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14548584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsub:	Enthalpy of sublimation 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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