Phenol, 2-methyl-4,6-dinitro, acetate

Other names: o-Cresol, 4,6-dinitro-, acetate
Inchi: InChI=1S/C9H8N2O6/c1-5-3-7(10(13)14)4-8(11(15)16)9(5)17-6(2)12/h3-4H,1-2H3
InchiKey: OEMKFZGDLXBFNO-UHFFFAOYSA-N
Formula: C9H8N2O6
SMILES: CC(=O)Oc1c(C)cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 240.17
CAS: 18461-55-7

Physical Properties

Property code	Value	Unit	Source
gf	-54.40	kJ/mol	Joback Method
hf	-293.29	kJ/mol	Joback Method
hfus	37.45	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	1.737		Crippen Method
mcvol	156.190	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1716.00		NIST Webbook
tb	826.91	K	Joback Method
tc	1088.15	K	Joback Method
tf	614.55	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.64	J/mol×K	826.91	Joback Method
cpg	434.75	J/mol×K	870.45	Joback Method
cpg	442.86	J/mol×K	913.99	Joback Method
cpg	449.98	J/mol×K	957.53	Joback Method
cpg	456.12	J/mol×K	1001.07	Joback Method
cpg	461.29	J/mol×K	1044.61	Joback Method
cpg	465.50	J/mol×K	1088.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18461557&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume