2,4-DINITROPHENYL ACETATE

Other names:	2,4-Dinitrophenyl acetate
	Phenol, 2,4-dinitro-, acetate
Inchi:	InChI=1S/C8H6N2O6/c1-5(11)16-8-3-2-6(9(12)13)4-7(8)10(14)15/h2-4H,1H3
InchiKey:	CDMLJWCAUSWULM-UHFFFAOYSA-N
Formula:	C8H6N2O6
SMILES:	CC(=O)Oc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	226.14

Physical Properties

Property code	Value	Unit	Source
hf	-265.35	kJ/mol	Cheméo Relay (1.0)
hfus	35.25	kJ/mol	Joback Method
hvap	83.07	kJ/mol	Cheméo Relay (1.0)
ie	9.72	eV	Cheméo Relay (1.0)
log10ws	-2.74		Cheméo Relay (1.0)
logp	1.428		Crippen Method
mcvol	142.100	ml/mol	McGowan Method
tb	551.27	K	Cheméo Relay (1.0)
tf	353.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.07	J/mol×K	799.05	Joback Method
cpg	384.68	J/mol×K	843.47	Joback Method
cpg	392.33	J/mol×K	887.89	Joback Method
cpg	399.02	J/mol×K	932.31	Joback Method
cpg	404.78	J/mol×K	976.73	Joback Method
cpg	409.62	J/mol×K	1021.15	Joback Method
cpg	413.57	J/mol×K	1065.57	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4232273&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point