Dinoseb acetate

Other names:	Phenol, 2-(1-methylpropyl)-4,6-dinitro-, acetate
	Acetic acid, 2-(sec-butyl)-4,6-dinitrophenyl ester
	Acetic acid, (2,4-dinitro-6-s-butylphenyl) ester
	Acetic acid, (4,6-dinitro-2-s-butylphenyl) ester
	O-Acetyl-2-sec-butyl-4,6-dinitrophenol
	Aretit
	2-sek.Butyl-4,6-dinitrofenylester kyseliny octove
	2-sec-Butyl-4,6-dinitrophenylacetate
	6-sec-Butyl-2,4-dinitrophenylacetate
	2,4-Dinitro-6-s-butylfenylester kyseliny octove
	2,4-Dinitro-6-sek.butyl-phenylacetat
	4,6-Dinitro-2-s-butylphenyl acetate
	Dinosebe acetate
	HOE 2904
	2-(2-Hydroxy-3,5-dinitrophenyl)butane acetate
	Ivosit
	2-(1-Methylpropyl)-4,6-dinitrophenyl acetate
	Phenol, 2-sec-butyl-4,6-dinitro-, acetate
	Phenol, 2-(1-methylpropyl)-4,6-dinitro-, acetate (ester)
	Phenol, 2-sec-butyl-4,6-dinitro-, acetate (ester)
Inchi:	InChI=1S/C12H14N2O6/c1-4-7(2)10-5-9(13(16)17)6-11(14(18)19)12(10)20-8(3)15/h5-7H
InchiKey:	RDJTWDKSYLLHRW-UHFFFAOYSA-N
Formula:	C12H14N2O6
SMILES:	CCC(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC(C)=O
Mol. weight [g/mol]:	282.25
CAS:	2813-95-8

Physical Properties

Property code	Value	Unit	Source
gf	-31.58	kJ/mol	Joback Method
hf	-360.49	kJ/mol	Joback Method
hfus	41.70	kJ/mol	Joback Method
hvap	88.52	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	2.942		Crippen Method
mcvol	198.460	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method

rinpol	1894.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	895.11	K	Joback Method
tc	1146.04	K	Joback Method
tf	633.36	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.38	J/mol×K	895.11	Joback Method
cpg	597.78	J/mol×K	936.93	Joback Method
cpg	607.02	J/mol×K	978.75	Joback Method
cpg	615.15	J/mol×K	1020.57	Joback Method
cpg	622.18	J/mol×K	1062.40	Joback Method
cpg	628.15	J/mol×K	1104.22	Joback Method
cpg	633.07	J/mol×K	1146.04	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=C2813958&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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