Dinobuton

Other names:	Carbonic acid, 1-methylethyl 2-(1-methylpropyl)-4,6-dinitrophenyl ester
	Carbonic acid, 2-sec-butyl-4,6-dinitrophenyl isopropyl ester
	Acrex
	Dessin
	Drawinol
	Isopropyl 2,4-dinitro-6-sec-butylphenyl carbonate
	Kasebon
	MC 1053
	Union Carbide 19786
	UC 19786
	2-sec-Butyl-4,6-dinitrophenyl isopropyl carbonate
	Sytasol
	2,4-Dinitro-6-sec-butylphenyl isopropyl carbonate
	Akrex
	Isophen (pesticide)
Inchi:	InChI=1S/C14H18N2O7/c1-5-9(4)11-6-10(15(18)19)7-12(16(20)21)13(11)23-14(17)22-8(
InchiKey:	HDWLUGYOLUHEMN-UHFFFAOYSA-N
Formula:	C14H18N2O7
SMILES:	CCC(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC(=O)OC(C)C
Mol. weight [g/mol]:	326.30
CAS:	973-21-7

Physical Properties

Property code	Value	Unit	Source
gf	-122.18	kJ/mol	Joback Method
hf	-539.27	kJ/mol	Joback Method
hfus	44.54	kJ/mol	Joback Method
hvap	94.99	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	3.940		Crippen Method
mcvol	232.510	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
tb	962.85	K	Joback Method
tc	1208.55	K	Joback Method
tf	663.13	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.38	J/mol×K	962.85	Joback Method
cpg	734.38	J/mol×K	1003.80	Joback Method
cpg	743.00	J/mol×K	1044.75	Joback Method
cpg	750.24	J/mol×K	1085.70	Joback Method
cpg	756.13	J/mol×K	1126.65	Joback Method
cpg	760.67	J/mol×K	1167.60	Joback Method
cpg	763.87	J/mol×K	1208.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C973217&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume