Dinocap

Other names:	2-Butenoic acid, 2(or 4)-isooctyl-4,6(or 2,6)-dinitrophenyl ester
	Caratan
	Carathane
	Crotothane
	Karatan
	Karathane
	Mancokar
	Mildex
	Arathane
	CR-1639
	DNOCP
	ENT-24727
	Isocothane
Inchi:	InChI=1S/C10H9NO4/c1-2-5-10(12)15-9-7-4-3-6-8(9)11(13)14/h2-7H,1H3/b5-2+
InchiKey:	RNDNTTTUTQAXII-GORDUTHDSA-N
Formula:	C18H24N2O6
SMILES:	CC=CC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	364.39
CAS:	39300-45-3

Physical Properties

Property code	Value	Unit	Source
gf	17.95	kJ/mol	Joback Method
hf	-163.01	kJ/mol	Joback Method
hfus	29.66	kJ/mol	Joback Method
hvap	66.50	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.076		Crippen Method
mcvol	148.560	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	692.15	K	Joback Method
tc	939.29	K	Joback Method
tf	452.09	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.69	J/mol×K	692.15	Joback Method
cpg	383.11	J/mol×K	733.34	Joback Method
cpg	393.60	J/mol×K	774.53	Joback Method
cpg	403.23	J/mol×K	815.72	Joback Method
cpg	412.03	J/mol×K	856.91	Joback Method
cpg	420.05	J/mol×K	898.10	Joback Method
cpg	427.33	J/mol×K	939.29	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=C39300453&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume