Pendimethalin

Other names:	Penoxaline
	Benzenamine, N-(1-ethylpropyl)-3,4-dimethyl-2,6-dinitro-
	Ac 92553
	Prowl
	Stomp
	Penoxalin
	Accotab
	Go-Go-San
	Herbadox
	Herbodox
	N-(1-Ethylpropyl)-3,4-dimethyl-2,6-dinitrobenzenamine
	Pre-M 60DG
	Prowl 3.3
	Prowl 4E
	Sipaxol
	Way Up
	Aniline, 3,4-dimethyl-2,6-dinitro-N-(1-ethylpropyl)-
	Pendimethaline
	3,4-Dimethyl-2,6-dinitro-N-(1-ethylpropyl)aniline
	N-(1-Ethylpropyl)-2,6-dinitro-3,4-xylidine
	Phenoxalin
	Southern Weed Grass Control
	Stomp 330D
	Stomp 330E
	SWGC
Inchi:	InChI=1S/C13H19N3O4/c1-5-10(6-2)14-12-11(15(17)18)7-8(3)9(4)13(12)16(19)20/h7,10
InchiKey:	CHIFOSRWCNZCFN-UHFFFAOYSA-N
Formula:	C13H19N3O4
SMILES:	CCC(CC)Nc1c([N+](=O)[O-])cc(C)c(C)c1[N+](=O)[O-]
Mol. weight [g/mol]:	281.31
CAS:	40487-42-1

Physical Properties

Property code	Value	Unit	Source
gf	290.52	kJ/mol	Joback Method
hf	-94.33	kJ/mol	Joback Method

hfus	46.21	kJ/mol	Joback Method
hvap	88.69	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	3.720		Crippen Method
mcvol	215.090	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2038.00		NIST Webbook
rinpol	1988.00		NIST Webbook
rinpol	2038.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2038.00		NIST Webbook
rinpol	2044.00		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
ripol	2768.00		NIST Webbook
tb	896.85	K	Joback Method
tc	1140.92	K	Joback Method
tf	327.85 ± 0.20	K	NIST Webbook
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.15	J/mol×K	896.85	Joback Method
cpg	672.42	J/mol×K	937.53	Joback Method
cpg	683.63	J/mol×K	978.21	Joback Method
cpg	693.82	J/mol×K	1018.88	Joback Method
cpg	703.05	J/mol×K	1059.56	Joback Method
cpg	711.37	J/mol×K	1100.24	Joback Method
cpg	718.82	J/mol×K	1140.92	Joback Method
hfust	25.19	kJ/mol	327.50	NIST Webbook

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=C40487421&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
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/44-914-8/Pendimethalin.pdf
Generated by Cheméo on 2024-04-26 17:22:22.738263872 +0000 UTC m=+16441391.658841184.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.