Dicamba

Other names:	2,5-Dichloro-6-methoxybenzoic acid
	2-Methoxy-3,6-dichlorobenzoic acid
	3,6-Dichloor-2-methoxy-benzoeizuur
	3,6-Dichlor-3-methoxy-benzoesaeure
	3,6-Dichloro-2-methoxybenzoic acid
	3,6-Dichloro-o-anisic acid
	Acido (3,6-dicloro-2-metossi)-benzoico
	Banlen
	Banvel
	Banvel 480
	Banvel 70WP
	Banvel CST
	Banvel II herbicide
	Banvel SGF
	Banvel herbicide
	Benzoic acid, 3,6-dichloro-2-methoxy-
	Brush buster
	Compound B dicamba
	Dianat
	Dianate
	Kyselina 3,6-dichlor-2-methoxybenzoova
	MDBA
	Mediben
	Vanquish
	Velsicol 58-CS-11
	Velsicol Compound "R"
	Velsicol compound R
	o-Anisic acid, 3,6-dichloro-
Inchi:	InChI=1S/C8H6Cl2O3/c1-13-7-5(10)3-2-4(9)6(7)8(11)12/h2-3H,1H3,(H,11,12)
InchiKey:	IWEDIXLBFLAXBO-UHFFFAOYSA-N
Formula:	C8H6Cl2O3
SMILES:	COc1c(Cl)ccc(Cl)c1C(=O)O
Mol. weight [g/mol]:	221.04
CAS:	1918-00-9

Physical Properties

Property code	Value	Unit	Source

gf	-294.60	kJ/mol	Joback Method
hf	-434.84	kJ/mol	Joback Method
hfus	24.62	kJ/mol	Joback Method
hvap	72.27	kJ/mol	Joback Method
log10ws	-1.70		Aqueous Solubility Prediction Method
logp	2.700		Crippen Method
mcvol	137.610	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
tb	667.39	K	Joback Method
tc	881.82	K	Joback Method
tf	386.50 ± 0.10	K	NIST Webbook
tf	387.23 ± 0.20	K	NIST Webbook
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.53	J/mol×K	881.82	Joback Method
cpg	328.39	J/mol×K	846.08	Joback Method
cpg	322.77	J/mol×K	810.35	Joback Method
cpg	316.68	J/mol×K	774.61	Joback Method
cpg	310.11	J/mol×K	738.87	Joback Method
cpg	303.07	J/mol×K	703.13	Joback Method
cpg	295.55	J/mol×K	667.39	Joback Method
dvisc	0.0009357	Pa×s	436.72	Joback Method
dvisc	0.0000648	Pa×s	667.39	Joback Method
dvisc	0.0000883	Pa×s	628.94	Joback Method
dvisc	0.0001251	Pa×s	590.50	Joback Method
dvisc	0.0001863	Pa×s	552.06	Joback Method
dvisc	0.0002944	Pa×s	513.61	Joback Method
dvisc	0.0005008	Pa×s	475.17	Joback Method
hfust	22.90	kJ/mol	386.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1918009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume