

Benzoic acid, 3,6-dichloro-2-methoxy-

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 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

Physical Properties

Property code	Value	Unit	Source
hfus	24.62	kJ/mol	Joback Method

log10ws	-1.70		Aqueous Solubility Prediction Method
logp	2.700		Crippen Method
mcvol	137.610	ml/mol	McGowan Method
rinpol	1617.00		NIST Webbook
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tf	387.23 ± 0.20	K	NIST Webbook
tf	386.50 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

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

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1918009&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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