Dicamba methyl ester

Other names:	Disugran
	Benzoic acid, 3,6-dichloro-2-methoxy-, methyl ester
	o-Anisic acid, 3,6-dichloro-, methyl ester
	Banvel 60CS16
	Methyl 2-methoxy-3,6-dichlorobenzoate
	Methyl 3,6-dichloro-o-anisate
	Methyl 3,6-dichloro-2-methoxybenzoate
	Racusa
	Racuza
	2-Methoxy-3,6-dichlorobenzoic acid methyl ester
	60CS16
	Benzoic acid, 3,6-dichloro-2-methoxy-, methylated
	Dicamba-methyl
Inchi:	InChI=1S/C9H8Cl2O3/c1-13-8-6(11)4-3-5(10)7(8)9(12)14-2/h3-4H,1-2H3
InchiKey:	AWSBKDYHGOOSML-UHFFFAOYSA-N
Formula:	C8H8Cl2O3
SMILES:	COC(=O)c1c(Cl)ccc(Cl)c1OC
Mol. weight [g/mol]:	223.05
CAS:	6597-78-0

Physical Properties

Property code	Value	Unit	Source
gf	-254.36	kJ/mol	Joback Method
hf	-435.47	kJ/mol	Joback Method
hfus	24.31	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.789		Crippen Method
mcvol	151.700	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
tb	620.51	K	Joback Method
tc	845.61	K	Joback Method
tf	305.14 ± 0.20	K	NIST Webbook
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.83	J/mol×K	620.51	Joback Method
cpg	334.03	J/mol×K	658.03	Joback Method
cpg	343.65	J/mol×K	695.54	Joback Method
cpg	352.69	J/mol×K	733.06	Joback Method
cpg	361.13	J/mol×K	770.57	Joback Method
cpg	368.94	J/mol×K	808.09	Joback Method
cpg	376.11	J/mol×K	845.61	Joback Method
dvisc	0.0005650	Pa×s	444.59	Joback Method
dvisc	0.0008111	Pa×s	409.40	Joback Method
dvisc	0.0004150	Pa×s	479.77	Joback Method
dvisc	0.0003179	Pa×s	514.96	Joback Method
dvisc	0.0002520	Pa×s	550.14	Joback Method
dvisc	0.0002054	Pa×s	585.33	Joback Method
dvisc	0.0001714	Pa×s	620.51	Joback Method
hfust	18.49	kJ/mol	304.60	NIST Webbook
hfust	18.49	kJ/mol	304.60	NIST Webbook
hfust	18.49	kJ/mol	304.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6597780&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

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