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

Other names: 2-Methoxy-3,6-dichlorobenzoic acid methyl ester
60CS16
Banvel 60CS16
Benzoic acid, 3,6-dichloro-2-methoxy-, methyl ester
Benzoic acid, 3,6-dichloro-2-methoxy-, methylated
Dicamba-methyl
Disugran
Methyl 2-methoxy-3,6-dichlorobenzoate
Methyl 3,6-dichloro-2-methoxybenzoate
Methyl 3,6-dichloro-o-anisate
Racusa
Racuza
o-Anisic acid, 3,6-dichloro-, methyl ester

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: C9H8Cl2O3

SMILES: COC(=O)c1c(Cl)ccc(Cl)c1OC

Mol. weight [g/mol]: 235.07

Physical Properties

Property code	Value	Unit	Source
hf	-472.51	kJ/mol	Cheméo Relay (1.0)
hfus	24.31	kJ/mol	Joback Method
hvap	77.34	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-3.53		Cheméo Relay (1.0)
logp	2.789		Crippen Method
mcvol	151.700	ml/mol	McGowan Method
tb	551.98	K	Cheméo Relay (1.0)
tf	305.14 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	368.94	J/mol×K	808.09	Joback Method
cpg	376.11	J/mol×K	845.61	Joback Method
cpg	361.13	J/mol×K	770.57	Joback Method
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
dvisc	0.0008111	Pa×s	409.40	Joback Method
dvisc	0.0005650	Pa×s	444.58	Joback Method
dvisc	0.0004150	Pa×s	479.77	Joback Method
dvisc	0.0003179	Pa×s	514.95	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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6597780&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point