Benzoic acid, 2,4-dichloro-, methyl ester

Other names:	Methyl ester of 2,4-Dichlorobenzoic acid
	Methyl 2,4-dichlorobenzoate
Inchi:	InChI=1S/C8H6Cl2O2/c1-12-8(11)6-3-2-5(9)4-7(6)10/h2-4H,1H3
InchiKey:	VCRWILYAWSRHBN-UHFFFAOYSA-N
Formula:	C8H6Cl2O2
SMILES:	COC(=O)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	205.04
CAS:	35112-28-8

Physical Properties

Property code	Value	Unit	Source
gf	-148.15	kJ/mol	Joback Method
hf	-271.14	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	54.93	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.780		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	570.23	K	Joback Method
tc	801.88	K	Joback Method
tf	363.38	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.56	J/mol×K	570.23	Joback Method
cpg	267.98	J/mol×K	608.84	Joback Method
cpg	276.81	J/mol×K	647.45	Joback Method
cpg	285.07	J/mol×K	686.06	Joback Method
cpg	292.76	J/mol×K	724.66	Joback Method
cpg	299.89	J/mol×K	763.27	Joback Method
cpg	306.45	J/mol×K	801.88	Joback Method

dvisc	0.0013093	Pa×s	363.38	Joback Method
dvisc	0.0008718	Pa×s	397.86	Joback Method
dvisc	0.0006194	Pa×s	432.33	Joback Method
dvisc	0.0004628	Pa×s	466.81	Joback Method
dvisc	0.0003600	Pa×s	501.28	Joback Method
dvisc	0.0002892	Pa×s	535.75	Joback Method
dvisc	0.0002386	Pa×s	570.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35112288&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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