Dichlorprop-methyl

Other names:	Propanoic acid, 2-(2',4'-dichlorophenoxy)-, methyl ester
	2,4-DP methyl ester
	Dichlorprop, methylated
	Dichlorprop, methyl ester
	Propanoic acid, 2-(2,4-dichlorophenoxy), methyl ester
	Propanoic acid, 2-(2,4-dichlorophenoxy)-, methyl ester, (.+/-.)-
	Methyl dichlorprop
Inchi:	InChI=1S/C10H10Cl2O3/c1-6(10(13)14-2)15-9-4-3-7(11)5-8(9)12/h3-6H,1-2H3
InchiKey:	SCHCPDWDIOTCMJ-UHFFFAOYSA-N
Formula:	C10H10Cl2O3
SMILES:	COC(=O)C(C)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	249.09
CAS:	57153-17-0

Physical Properties

Property code	Value	Unit	Source
gf	-238.75	kJ/mol	Joback Method
hf	-449.92	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	61.40	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.934		Crippen Method
mcvol	165.790	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1574.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1593.00		NIST Webbook
ripol	2242.00		NIST Webbook
ripol	2241.00		NIST Webbook
tb	637.97	K	Joback Method
tc	862.55	K	Joback Method
tf	393.15	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.78	J/mol×K	637.97	Joback Method
cpg	423.27	J/mol×K	825.12	Joback Method
cpg	414.63	J/mol×K	787.69	Joback Method
cpg	405.26	J/mol×K	750.26	Joback Method
cpg	395.15	J/mol×K	712.83	Joback Method
cpg	384.33	J/mol×K	675.40	Joback Method
cpg	431.17	J/mol×K	862.55	Joback Method
dvisc	0.0001454	Pa×s	637.97	Joback Method
dvisc	0.0001812	Pa×s	597.17	Joback Method
dvisc	0.0002332	Pa×s	556.36	Joback Method
dvisc	0.0003123	Pa×s	515.56	Joback Method
dvisc	0.0004398	Pa×s	474.76	Joback Method
dvisc	0.0006605	Pa×s	433.95	Joback Method
dvisc	0.0010795	Pa×s	393.15	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57153170&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume