PROPANOIC ACID, 2-(2,4-DICHLOROPHENOXY)-, METHYL ESTER

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

Physical Properties

Property code	Value	Unit	Source
hfus	23.77	kJ/mol	Joback Method
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-3.06		Cheméo Relay (1.0)
logp	2.934		Crippen Method
mcvol	165.790	ml/mol	McGowan Method
rinpol	1576.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1574.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2242.00		NIST Webbook
tb	534.24	K	Cheméo Relay (1.0)
tf	329.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.78	J/mol×K	637.97	Joback Method
cpg	384.33	J/mol×K	675.40	Joback Method

cpg	395.15	J/mol×K	712.83	Joback Method
cpg	405.26	J/mol×K	750.26	Joback Method
cpg	414.63	J/mol×K	787.69	Joback Method
cpg	423.27	J/mol×K	825.12	Joback Method
cpg	431.17	J/mol×K	862.55	Joback Method
dvisc	0.0010795	Pa×s	393.15	Joback Method
dvisc	0.0006605	Pa×s	433.95	Joback Method
dvisc	0.0004398	Pa×s	474.76	Joback Method
dvisc	0.0003123	Pa×s	515.56	Joback Method
dvisc	0.0002332	Pa×s	556.36	Joback Method
dvisc	0.0001812	Pa×s	597.17	Joback Method
dvisc	0.0001454	Pa×s	637.97	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57153170&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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