2,4-D, propyl ester

Other names:	propyl 2,4-dichlorophenoxyacetate
	2,4-Dichlorophenoxyacetic acid, propyl ester
Inchi:	InChI=1S/C11H12Cl2O3/c1-2-5-15-11(14)7-16-10-4-3-8(12)6-9(10)13/h3-4,6H,2,5,7H2,1
InchiKey:	URELEWKDONECLX-UHFFFAOYSA-N
Formula:	C11H12Cl2O3
SMILES:	CCCOC(=O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	263.12
CAS:	1928-61-6

Physical Properties

Property code	Value	Unit	Source
gf	-227.89	kJ/mol	Joback Method
hf	-465.28	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.325		Crippen Method
mcvol	179.880	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
tb	661.29	K	Joback Method
tc	877.62	K	Joback Method
tf	419.42	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.93	J/mol×K	661.29	Joback Method
cpg	432.96	J/mol×K	697.35	Joback Method
cpg	444.25	J/mol×K	733.40	Joback Method
cpg	454.81	J/mol×K	769.46	Joback Method
cpg	464.62	J/mol×K	805.51	Joback Method
cpg	473.70	J/mol×K	841.57	Joback Method
cpg	482.04	J/mol×K	877.62	Joback Method

dvisc	0.0008811	Pa×s	419.42	Joback Method
dvisc	0.0005668	Pa×s	459.73	Joback Method
dvisc	0.0003915	Pa×s	500.04	Joback Method
dvisc	0.0002858	Pa×s	540.36	Joback Method
dvisc	0.0002179	Pa×s	580.67	Joback Method
dvisc	0.0001721	Pa×s	620.98	Joback Method
dvisc	0.0001399	Pa×s	661.29	Joback Method
hvapt	77.30	kJ/mol	508.50	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1928616&Units=SI

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
hvapt: Enthalpy of vaporization at a given temperature
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

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