2,4-D Pentyl ester

Other names:	pentyl (2,4-dichlorophenoxy)acetate
	Acetic acid, 2-(2,4-dichlorophenoxy)-, pentyl ester
Inchi:	InChI=1S/C13H16Cl2O3/c1-2-3-4-7-17-13(16)9-18-12-6-5-10(14)8-11(12)15/h5-6,8H,2-4
InchiKey:	VZCCHPAEDSPPDG-UHFFFAOYSA-N
Formula:	C13H16Cl2O3
SMILES:	CCCCCOC(=O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	291.17
CAS:	1917-92-6

Physical Properties

Property code	Value	Unit	Source
gf	-211.05	kJ/mol	Joback Method
hf	-506.56	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.106		Crippen Method
mcvol	208.060	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
tb	707.05	K	Joback Method
tc	916.94	K	Joback Method
tf	441.96	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.62	J/mol×K	707.05	Joback Method
cpg	535.83	J/mol×K	742.03	Joback Method
cpg	548.22	J/mol×K	777.01	Joback Method
cpg	559.78	J/mol×K	812.00	Joback Method
cpg	570.52	J/mol×K	846.98	Joback Method
cpg	580.44	J/mol×K	881.96	Joback Method
cpg	589.55	J/mol×K	916.94	Joback Method

dvisc	0.0007759	Pa×s	441.96	Joback Method
dvisc	0.0004836	Pa×s	486.14	Joback Method
dvisc	0.0003262	Pa×s	530.32	Joback Method
dvisc	0.0002337	Pa×s	574.50	Joback Method
dvisc	0.0001756	Pa×s	618.69	Joback Method
dvisc	0.0001371	Pa×s	662.87	Joback Method
dvisc	0.0001104	Pa×s	707.05	Joback Method
hvapt	73.60	kJ/mol	508.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1917926&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
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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