N-propyl ester of 2,4,5-trichlorophenoxy acetic acid

Other names: 2,4,5-T, propyl ester
propyl 2,4,5-trichlorophenoxyacetate
2,4,5-Trichlorophenoxyacetic acid, propyl ester
Inchi: InChI=1S/C11H11Cl3O3/c1-2-3-16-11(15)6-17-10-5-8(13)7(12)4-9(10)14/h4-5H,2-3,6H2
InchiKey: KQPZLIOOEZZUFO-UHFFFAOYSA-N
Formula: C11H11Cl3O3
SMILES: CCCOC(=O)COc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 297.56
CAS: 1928-40-1

Physical Properties

Property code	Value	Unit	Source
gf	-249.45	kJ/mol	Joback Method
hf	-492.49	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.979		Crippen Method
mcvol	192.120	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	703.70	K	Joback Method
tc	924.00	K	Joback Method
tf	461.86	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.67	J/mol×K	703.70	Joback Method
cpg	453.65	J/mol×K	740.42	Joback Method
cpg	463.90	J/mol×K	777.13	Joback Method
cpg	473.41	J/mol×K	813.85	Joback Method
cpg	482.17	J/mol×K	850.57	Joback Method
cpg	490.19	J/mol×K	887.28	Joback Method

cpg	497.44	J/mol×K	924.00	Joback Method
dvisc	0.0006663	Pa×s	461.86	Joback Method
dvisc	0.0004523	Pa×s	502.17	Joback Method
dvisc	0.0003251	Pa×s	542.47	Joback Method
dvisc	0.0002447	Pa×s	582.78	Joback Method
dvisc	0.0001910	Pa×s	623.09	Joback Method
dvisc	0.0001537	Pa×s	663.39	Joback Method
dvisc	0.0001268	Pa×s	703.70	Joback Method
hvapt	83.20	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=C1928401&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