

2,4,5-T, ethyl ester

Other names:	ethyl 2,4,5-trichlorophenoxyacetate (2,4,5-Trichlorophenoxy)acetic acid, ethyl ester
Inchi:	InChI=1S/C10H9Cl3O3/c1-2-15-10(14)5-16-9-4-7(12)6(11)3-8(9)13/h3-4H,2,5H2,1H3
InchiKey:	LVNNFHCEDQSWSC-UHFFFAOYSA-N
Formula:	C10H9Cl3O3
SMILES:	CCOC(=O)COc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	283.54
CAS:	1928-39-8

Physical Properties

Property code	Value	Unit	Source
gf	-257.87	kJ/mol	Joback Method
hf	-471.85	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	66.84	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.589		Crippen Method
mcvol	178.030	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	680.82	K	Joback Method
tc	904.94	K	Joback Method
tf	450.59	K	Joback Method
vc	0.676	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.44	J/molxK	904.94	Joback Method
cpg	437.65	J/molxK	867.58	Joback Method
cpg	430.14	J/molxK	830.23	Joback Method
cpg	421.92	J/molxK	792.88	Joback Method
cpg	413.01	J/molxK	755.53	Joback Method
cpg	403.41	J/molxK	718.17	Joback Method
cpg	393.14	J/molxK	680.82	Joback Method

dvisc	0.0007093	Paxs	450.59	Joback Method
dvisc	0.0001428	Paxs	680.82	Joback Method
dvisc	0.0001722	Paxs	642.45	Joback Method
dvisc	0.0002127	Paxs	604.08	Joback Method
dvisc	0.0002703	Paxs	565.71	Joback Method
dvisc	0.0003558	Paxs	527.33	Joback Method
dvisc	0.0004890	Paxs	488.96	Joback Method
hvapt	76.40	kJ/mol	508.50	NIST Webbook

Sources

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=C1928398&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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