2,4,5-T Methyl ester

Other names:	2,4,5-Trichlorophenoxyacetic acid methyl ester
	Acetic acid, (2,4,5-trichlorophenoxy)-, methyl ester
	Acetic acid, (2,4,5-trichlorophenoxy)-, methylated
	Methyl (2,4,5-trichlorophenoxy)acetate
Inchi:	InChI=1S/C9H7Cl3O3/c1-14-9(13)4-15-8-3-6(11)5(10)2-7(8)12/h2-3H,4H2,1H3
InchiKey:	JUCNGUOYQGHBJC-UHFFFAOYSA-N
Formula:	C9H7Cl3O3
SMILES:	COC(=O)COc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	269.51
CAS:	1928-37-6

Physical Properties

Property code	Value	Unit	Source
gf	-266.29	kJ/mol	Joback Method
hf	-451.21	kJ/mol	Joback Method
hfus	28.51	kJ/mol	Joback Method
hvap	64.61	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.199		Crippen Method
mcvol	163.940	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
ripol	2551.00		NIST Webbook
ripol	2552.00		NIST Webbook
ripol	2551.00		NIST Webbook
tb	657.94	K	Joback Method
tc	886.25	K	Joback Method
tf	363.10 ± 0.20	K	NIST Webbook
tf	363.35 ± 0.20	K	NIST Webbook
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.04	J/mol×K	848.20	Joback Method
cpg	371.56	J/mol×K	772.10	Joback Method
cpg	363.36	J/mol×K	734.04	Joback Method
cpg	354.53	J/mol×K	695.99	Joback Method
cpg	345.09	J/mol×K	657.94	Joback Method
cpg	379.13	J/mol×K	810.15	Joback Method
cpg	392.29	J/mol×K	886.25	Joback Method
dvisc	0.0007498	Pa×s	439.32	Joback Method
dvisc	0.0001601	Pa×s	657.94	Joback Method
dvisc	0.0001920	Pa×s	621.50	Joback Method
dvisc	0.0002356	Pa×s	585.07	Joback Method
dvisc	0.0002970	Pa×s	548.63	Joback Method
dvisc	0.0003871	Pa×s	512.19	Joback Method
dvisc	0.0005253	Pa×s	475.76	Joback Method
hfust	31.95	kJ/mol	360.60	NIST Webbook
hfust	30.46	kJ/mol	361.90	NIST Webbook
hvapt	76.90	kJ/mol	508.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.21293e+01
Coeff. B	-3.07775e+03
Coeff. C	-1.94000e+02
Temperature range (K), min.	444.00
Temperature range (K), max.	645.43

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=C1928376&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume