2,4-D methyl ester

Other names:	(2,4-Dichlorophenoxy)acetic acid, methyl ester
	Acetic acid, (2,4-dichlorophenoxy)-, methyl ester
	Acetic acid, (2,4-dichlorophenoxy)-, methylated
	D (2,4-) methylester
	Methyl (2,4-dichlorophenoxy)acetate
	Methyl 2,4-D ester
	Methyl ester of 2,4-Dichlorophenoxyacetic acid
	ethanoic acid, 2,4-dichlorophenoxy-, methyl ester
	methyl 2,4-dichlorophenoxyacetate
	methyl 2,4-dichlorophenoxyethanoate
Inchi:	InChI=1S/C9H8Cl2O3/c1-13-9(12)5-14-8-3-2-6(10)4-7(8)11/h2-4H,5H2,1H3
InchiKey:	HWIGZMADSFQMOI-UHFFFAOYSA-N
Formula:	C9H8Cl2O3
SMILES:	COC(=O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	235.06
CAS:	1928-38-7

Physical Properties

Property code	Value	Unit	Source
gf	-244.73	kJ/mol	Joback Method
hf	-424.00	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	59.56	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.545		Crippen Method
mcvol	151.700	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1590.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1605.00		NIST Webbook
ripol	2465.00		NIST Webbook

ripol	2396.00		NIST Webbook
ripol	2395.00		NIST Webbook
ripol	2465.00		NIST Webbook
ripol	2395.00		NIST Webbook
tb	615.53	K	Joback Method
tc	839.68	K	Joback Method
tf	315.40 ± 0.20	K	NIST Webbook
tf	310.70	K	Standard Sublimation Enthalpies of some dichlorophenoxy acids and their methyl esters
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.49	J/mol×K	727.60	Joback Method
cpg	378.14	J/mol×K	839.68	Joback Method
cpg	370.91	J/mol×K	802.32	Joback Method
cpg	363.02	J/mol×K	764.96	Joback Method
cpg	325.15	J/mol×K	615.53	Joback Method
cpg	335.55	J/mol×K	652.89	Joback Method
cpg	345.33	J/mol×K	690.25	Joback Method
dvisc	0.0001737	Pa×s	615.53	Joback Method
dvisc	0.0003410	Pa×s	506.20	Joback Method
dvisc	0.0002642	Pa×s	542.65	Joback Method
dvisc	0.0002115	Pa×s	579.09	Joback Method
dvisc	0.0009703	Pa×s	396.88	Joback Method
dvisc	0.0006457	Pa×s	433.32	Joback Method
dvisc	0.0004578	Pa×s	469.76	Joback Method
hfust	25.10	kJ/mol	315.40	NIST Webbook
hfust	25.10	kJ/mol	315.40	NIST Webbook
hfust	20.00	kJ/mol	313.40	NIST Webbook
hvapt	68.00	kJ/mol	475.50	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42863e+01
Coeff. B	-5.28300e+03
Coeff. C	-6.24900e+01
Temperature range (K), min.	403.00
Temperature range (K), max.	651.14

Sources

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=C1928387&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Standard Sublimation Enthalpies of some dichlorophenoxy acids and their methyl esters:	https://www.doi.org/10.1021/je049626l

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