Swep

Other names:	Carbamic acid, (3,4-dichlorophenyl)-, methyl ester
	Carbanilic acid, 3,4-dichloro-, methyl ester
	Methyl N-(3,4-dichlorophenyl)carbamate
	Methyl 3,4-dichlorocarbanilate
	Methyl 3,4-dichlorophenylcarbamate
	MCC
	NIA 2,995
	3,4-Dichlorocarbanilic acid methyl ester
	FMC 2995
	Methylester kyseliny 3,4-dichlorkarbanilove
	NIA 2995J
	3,4-Dichlorophenylcarbamic acid methyl ester
Inchi:	InChI=1S/C8H7Cl2NO2/c1-13-8(12)11-5-2-3-6(9)7(10)4-5/h2-4H,1H3,(H,11,12)
InchiKey:	WOZQBERUBLYCEG-UHFFFAOYSA-N
Formula:	C8H7Cl2NO
SMILES:	COC(=O)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	204.05
CAS:	1918-18-9

Physical Properties

Property code	Value	Unit	Source
gf	-58.76	kJ/mol	Joback Method
hf	-217.67	kJ/mol	Joback Method
hfus	26.02	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.172		Crippen Method
mcvol	141.720	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
ripol	2947.00		NIST Webbook
tb	620.40	K	Joback Method
tc	850.53	K	Joback Method
tf	382.70 ± 0.20	K	NIST Webbook
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.26	J/mol×K	773.82	Joback Method
cpg	342.35	J/mol×K	812.18	Joback Method
cpg	300.55	J/mol×K	620.40	Joback Method
cpg	310.19	J/mol×K	658.76	Joback Method
cpg	319.18	J/mol×K	697.11	Joback Method
cpg	327.53	J/mol×K	735.47	Joback Method
cpg	348.84	J/mol×K	850.53	Joback Method
hfust	23.19	kJ/mol	381.40	NIST Webbook
hfust	23.19	kJ/mol	381.40	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=C1918189&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical 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