Acetic acid, (2,4,5-trichlorophenoxy)-, 2-methylpropyl ester

Other names: Acetic acid, (2,4,5-trichlorophenoxy)-, isobutyl ester
Isobutyl 2,4,5-T
2,4,5-t Isobutyl ester
isobutyl 2,4,5-trichlorophenoxyacetate

Inchi: InChI=1S/C12H13Cl3O3/c1-7(2)5-18-12(16)6-17-11-4-9(14)8(13)3-10(11)15/h3-4,7H,5-6

InchiKey: KIIVFWSIMRWBKW-UHFFFAOYSA-N

Formula: C12H13Cl3O3

SMILES: CC(C)COC(=O)COc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 311.59

CAS: 4938-72-1

Physical Properties

Property code	Value	Unit	Source
gf	-243.47	kJ/mol	Joback Method
hf	-518.41	kJ/mol	Joback Method
hfus	32.75	kJ/mol	Joback Method
hvap	70.90	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.225		Crippen Method
mcvol	206.210	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
tb	726.14	K	Joback Method
tc	946.85	K	Joback Method
tf	458.13	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.15	J/mol×K	726.14	Joback Method
cpg	505.96	J/mol×K	762.93	Joback Method
cpg	516.94	J/mol×K	799.71	Joback Method
cpg	527.10	J/mol×K	836.50	Joback Method
cpg	536.43	J/mol×K	873.28	Joback Method

cpg	544.92	J/mol×K	910.07	Joback Method
cpg	552.57	J/mol×K	946.85	Joback Method
dvisc	0.0006939	Pa×s	458.13	Joback Method
dvisc	0.0004389	Pa×s	502.80	Joback Method
dvisc	0.0002991	Pa×s	547.47	Joback Method
dvisc	0.0002160	Pa×s	592.13	Joback Method
dvisc	0.0001633	Pa×s	636.80	Joback Method
dvisc	0.0001281	Pa×s	681.47	Joback Method
dvisc	0.0001035	Pa×s	726.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4938721&Units=SI
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

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
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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