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

Other names: (2,4,5-Trichlorophenoxy)acetic acid butyl ester
2,4,5-T Butyl ester
2,4,5-T n-Butyl ester
Arboricid
Butyl (2,4,5-trichlorophenoxy)acetate
Butyl 2,4,5-T
Butylate 2,4,5-T
Flomore
Kilex 3
Krzewotoks
Krzewotox
NSC 190448
Tormona
Trioxone
U 46KW
n-Butyl (2,4,5-trichlorophenoxy)acetate
n-Butylester kyselini 2,4,5-trichlorfenoxyoctove

Inchi: InChI=1S/C12H13Cl3O3/c1-2-3-4-17-12(16)7-18-11-6-9(14)8(13)5-10(11)15/h5-6H,2-4,7

InchiKey: FNEXNZUHBCBQTI-UHFFFAOYSA-N

Formula: C12H13Cl3O3

SMILES: CCCCOC(=O)COc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 311.59

CAS: 93-79-8

Physical Properties

Property code	Value	Unit	Source
gf	-241.03	kJ/mol	Joback Method
hf	-513.13	kJ/mol	Joback Method
hfus	36.28	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.369		Crippen Method
mcvol	206.210	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
tb	726.58	K	Joback Method
tc	943.48	K	Joback Method
tf	473.13	K	Joback Method

vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.27	J/mol×K	943.48	Joback Method
cpg	493.56	J/mol×K	726.58	Joback Method
cpg	505.15	J/mol×K	762.73	Joback Method
cpg	515.96	J/mol×K	798.88	Joback Method
cpg	525.97	J/mol×K	835.03	Joback Method
cpg	535.20	J/mol×K	871.18	Joback Method
cpg	543.63	J/mol×K	907.33	Joback Method
dvisc	0.0001121	Pa×s	726.58	Joback Method
dvisc	0.0006220	Pa×s	473.13	Joback Method
dvisc	0.0004158	Pa×s	515.37	Joback Method
dvisc	0.0002955	Pa×s	557.61	Joback Method
dvisc	0.0002203	Pa×s	599.86	Joback Method
dvisc	0.0001707	Pa×s	642.10	Joback Method
dvisc	0.0001365	Pa×s	684.34	Joback Method
hvapt	87.30	kJ/mol	516.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25662e+01
Coeff. B	-3.14123e+03
Coeff. C	-2.14920e+02
Temperature range (K), min.	460.00
Temperature range (K), max.	647.91

Sources

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
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=C93798&Units=SI

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume