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

Other names: n-Butyl ester of alpha-(2,4,5-trichlorophenoxy)propionic acid
2,4,5-TP, butyl ester
Fenoprop, butyl ester
butyl 2-(2,4,5-trichlorophenoxy)propionate

Inchi: InChI=1S/C13H15Cl3O3/c1-3-4-5-18-13(17)8(2)19-12-7-10(15)9(14)6-11(12)16/h6-8H,3-

InchiKey: VPXVRVAKKVBOLA-UHFFFAOYSA-N

Formula: C13H15Cl3O3

SMILES: CCCCOC(=O)C(C)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 325.62

CAS: 13557-98-7

Physical Properties

Property code	Value	Unit	Source
gf	-235.05	kJ/mol	Joback Method
hf	-539.05	kJ/mol	Joback Method
hfus	35.34	kJ/mol	Joback Method
hvap	73.13	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.757		Crippen Method
mcvol	220.300	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	2035.00		NIST Webbook
rinpol	2035.00		NIST Webbook
tb	749.02	K	Joback Method
tc	966.49	K	Joback Method
tf	469.40	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.32	J/mol×K	749.02	Joback Method
cpg	558.64	J/mol×K	785.27	Joback Method
cpg	570.08	J/mol×K	821.51	Joback Method

cpg	580.66	J/mol×K	857.76	Joback Method
cpg	590.36	J/mol×K	894.00	Joback Method
cpg	599.19	J/mol×K	930.25	Joback Method
cpg	607.15	J/mol×K	966.49	Joback Method
dvisc	0.0006417	Pa×s	469.40	Joback Method
dvisc	0.0004000	Pa×s	516.00	Joback Method
dvisc	0.0002697	Pa×s	562.61	Joback Method
dvisc	0.0001931	Pa×s	609.21	Joback Method
dvisc	0.0001450	Pa×s	655.81	Joback Method
dvisc	0.0001131	Pa×s	702.42	Joback Method
dvisc	0.0000910	Pa×s	749.02	Joback Method

Sources

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=C13557987&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume