Butanoic acid, 4-(2,4,5-trichlorophenoxy)-, methyl ester

Other names: Butyric acid, 4-(2,4,5-trichlorophenoxy)-, methyl ester
Methyl 4-(2,4,5-trichlorophenoxy)butyrate
4-(2,4,5-Trichlorophenoxy)butyric acid methyl ester
Methyl 4-(2,4,5-trichlorophenoxy)butanoate
2,4,5-TB methyl ester
4-(2,4,5-TB) methyl ester

Inchi: InChI=1S/C11H11Cl3O3/c1-16-11(15)3-2-4-17-10-6-8(13)7(12)5-9(10)14/h5-6H,2-4H2,1

InchiKey: OTBMAATXBNOQHO-UHFFFAOYSA-N

Formula: C11H11Cl3O3

SMILES: COC(=O)CCCOc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 297.56

CAS: 25333-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-249.45	kJ/mol	Joback Method
hf	-492.49	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.979		Crippen Method
mcvol	192.120	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
ripol	2720.00		NIST Webbook
ripol	2720.00		NIST Webbook
ripol	2720.00		NIST Webbook
tb	703.70	K	Joback Method
tc	924.00	K	Joback Method
tf	461.86	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.67	J/mol×K	703.70	Joback Method
cpg	453.65	J/mol×K	740.42	Joback Method
cpg	463.90	J/mol×K	777.13	Joback Method
cpg	473.41	J/mol×K	813.85	Joback Method
cpg	482.17	J/mol×K	850.57	Joback Method
cpg	490.19	J/mol×K	887.28	Joback Method
cpg	497.44	J/mol×K	924.00	Joback Method
dvisc	0.0006663	Pa×s	461.86	Joback Method
dvisc	0.0004523	Pa×s	502.17	Joback Method
dvisc	0.0003251	Pa×s	542.47	Joback Method
dvisc	0.0002447	Pa×s	582.78	Joback Method
dvisc	0.0001910	Pa×s	623.09	Joback Method
dvisc	0.0001537	Pa×s	663.39	Joback Method
dvisc	0.0001268	Pa×s	703.70	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25333215&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
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