Butanoic acid, 4-[(2,4-dichlorophenyl)oxy]-, butyl ester

Other names: 2,4-DB butyl ester
Butanoic acid, 4-(2,4-dichlorophenoxy)-, butyl ester
Butyric acid, 4-(2,4-dichlorophenoxy)-, butyl ester
4-(2,4-Dichlorophenoxy)butyric acid butyl ester
butyl 4-(2,4-dichlorophenoxy)butyrate

Inchi: InChI=1S/C14H18Cl2O3/c1-2-3-8-19-14(17)5-4-9-18-13-7-6-11(15)10-12(13)16/h6-7,10H

InchiKey: IXXKVXJYFVAQBI-UHFFFAOYSA-N

Formula: C14H18Cl2O3

SMILES: CCCCOC(=O)CCCOc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 305.20

CAS: 6753-24-8

Physical Properties

Property code	Value	Unit	Source
gf	-202.63	kJ/mol	Joback Method
hf	-527.20	kJ/mol	Joback Method
hfus	37.65	kJ/mol	Joback Method
hvap	70.69	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.496		Crippen Method
mcvol	222.150	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
tb	729.93	K	Joback Method
tc	937.23	K	Joback Method
tf	453.23	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.43	J/mol×K	729.93	Joback Method
cpg	589.12	J/mol×K	764.48	Joback Method
cpg	601.93	J/mol×K	799.03	Joback Method
cpg	613.87	J/mol×K	833.58	Joback Method

cpg	624.96	J/mol×K	868.13	Joback Method
cpg	635.21	J/mol×K	902.68	Joback Method
cpg	644.61	J/mol×K	937.23	Joback Method
dvisc	0.0007209	Pa×s	453.23	Joback Method
dvisc	0.0004427	Pa×s	499.35	Joback Method
dvisc	0.0002953	Pa×s	545.46	Joback Method
dvisc	0.0002097	Pa×s	591.58	Joback Method
dvisc	0.0001566	Pa×s	637.70	Joback Method
dvisc	0.0001216	Pa×s	683.81	Joback Method
dvisc	0.0000974	Pa×s	729.93	Joback Method

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=C6753248&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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