Butanoic acid, 4-(2,4-dichlorophenoxy)-, methyl ester

Other names: 2,4-DB methyl ester
4-(2,4-Dichlorophenoxy)butyric acid methyl ester
Butanoic acid, 4-(2,4-dichlorophenoxy)-, methylated
Butyric acid, 4-(2,4-dichlorophenoxy)-, methyl ester
DB (2,4)-Methyl
Methyl 4-(2,4-dichlorophenoxy)butanoate
Methyl 4-(2,4-dichlorophenoxy)butyrate

Inchi: InChI=1S/C11H12Cl2O3/c1-15-11(14)3-2-6-16-10-5-4-8(12)7-9(10)13/h4-5,7H,2-3,6H2,1

InchiKey: NKXSNMCGZZWMMW-UHFFFAOYSA-N

Formula: C11H12Cl2O3

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

Mol. weight [g/mol]: 263.12

CAS: 18625-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-227.89	kJ/mol	Joback Method
hf	-465.28	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.325		Crippen Method
mcvol	179.880	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1794.00		NIST Webbook
rinpol	1799.00		NIST Webbook
ripol	2551.00		NIST Webbook
ripol	2552.00		NIST Webbook
tb	661.29	K	Joback Method
tc	877.62	K	Joback Method
tf	308.10	K	Standard Sublimation Enthalpies of some dichlorophenoxy acids and their methyl esters
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.62	J/mol×K	805.51	Joback Method
cpg	482.04	J/mol×K	877.62	Joback Method
cpg	473.70	J/mol×K	841.57	Joback Method
cpg	420.93	J/mol×K	661.29	Joback Method
cpg	432.96	J/mol×K	697.35	Joback Method
cpg	444.25	J/mol×K	733.40	Joback Method
cpg	454.81	J/mol×K	769.46	Joback Method
dvisc	0.0001399	Pa×s	661.29	Joback Method
dvisc	0.0002179	Pa×s	580.67	Joback Method
dvisc	0.0001721	Pa×s	620.98	Joback Method
dvisc	0.0008811	Pa×s	419.42	Joback Method
dvisc	0.0005668	Pa×s	459.73	Joback Method
dvisc	0.0003915	Pa×s	500.04	Joback Method
dvisc	0.0002858	Pa×s	540.36	Joback Method
hfust	32.64	kJ/mol	309.60	NIST Webbook
hfust	32.64	kJ/mol	309.60	NIST Webbook
hfust	22.00	kJ/mol	309.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18625122&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Standard Sublimation Enthalpies of some dichlorophenoxy acids and their methyl esters: https://www.doi.org/10.1021/je049626l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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