Acetic acid, (2,4-dichlorophenoxy)-, 2-methylpropyl ester

Other names: 2,4-D isobutyl ester
Acetic acid, (2,4-dichlorophenoxy)-, isobutyl ester
Isobutyl 2,4-dichlorophenoxyacetate
Isobutyl 2,4-d
2,4-Dichlorophenoxyacetic acid isobutyl ester
D (2,4-) isobutylester

Inchi: InChI=1S/C12H14Cl2O3/c1-8(2)6-17-12(15)7-16-11-4-3-9(13)5-10(11)14/h3-5,8H,6-7H2

InchiKey: GPSGZZSRFJXXBA-UHFFFAOYSA-N

Formula: C12H14Cl2O3

SMILES: CC(C)COC(=O)COc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 277.14

CAS: 1713-15-1

Physical Properties

Property code	Value	Unit	Source
gf	-221.91	kJ/mol	Joback Method
hf	-491.20	kJ/mol	Joback Method
hfus	28.95	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.571		Crippen Method
mcvol	193.970	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1805.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1805.00		NIST Webbook
tb	683.73	K	Joback Method
tc	900.59	K	Joback Method
tf	415.69	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	471.63	J/mol×K	683.73	Joback Method
cpg	528.05	J/mol×K	864.44	Joback Method
cpg	518.41	J/mol×K	828.30	Joback Method
cpg	507.95	J/mol×K	792.16	Joback Method
cpg	496.67	J/mol×K	756.02	Joback Method
cpg	484.56	J/mol×K	719.87	Joback Method
cpg	536.86	J/mol×K	900.59	Joback Method
dvisc	0.0001154	Pa×s	683.73	Joback Method
dvisc	0.0001451	Pa×s	639.06	Joback Method
dvisc	0.0001889	Pa×s	594.38	Joback Method
dvisc	0.0002567	Pa×s	549.71	Joback Method
dvisc	0.0003682	Pa×s	505.04	Joback Method
dvisc	0.0005664	Pa×s	460.36	Joback Method
dvisc	0.0009560	Pa×s	415.69	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=C1713151&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume