(2,3,5,6-Tetrafluorophenyl)methyl 3-(2,2-dichlorovinyl)-2,2-dimethyl-cyclopropane-1

Other names: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (2,3,5,6-tetrafluorophenyl)methyl ester
Bayothrin
Transfluthrin

Inchi: InChI=1S/C15H12Cl2F4O2/c1-15(2)7(3-10(16)17)11(15)14(22)23-5-6-12(20)8(18)4-9(19

InchiKey: DDVNRFNDOPPVQJ-UHFFFAOYSA-N

Formula: C15H12Cl2F4O2

SMILES: CC1(C)C(C=C(Cl)Cl)C1C(=O)OCc1c(F)c(F)cc(F)c1F

Mol. weight [g/mol]: 371.15

CAS: 118712-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-776.20	kJ/mol	Joback Method
hf	-1068.21	kJ/mol	Joback Method
hfus	43.46	kJ/mol	Joback Method
hvap	66.75	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.877		Crippen Method
mcvol	222.290	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	1910.00		NIST Webbook
tb	739.11	K	Joback Method
tc	943.26	K	Joback Method
tf	483.99	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.85	J/mol×K	739.11	Joback Method
cpg	605.59	J/mol×K	773.13	Joback Method
cpg	617.89	J/mol×K	807.16	Joback Method
cpg	629.85	J/mol×K	841.18	Joback Method
cpg	641.58	J/mol×K	875.21	Joback Method

cpg	653.19	J/mol×K	909.23	Joback Method
cpg	664.78	J/mol×K	943.26	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=C118712893&Units=SI

Legend

cpg:	Ideal gas heat capacity
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