Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester, cis-

Other names:	cis-Permethrin Permethrin-(cis) m-phenoxybenzyl cis-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate (3-Phenoxyphenyl)methyl-cis-3-(2,2-dichloroethenyl-2,2-dimethylcyclopropanecarboxylat (cis-permethrin)
Inchi:	InChI=1S/C21H20Cl2O3/c1-21(2)17(12-18(22)23)19(21)20(24)25-13-14-7-6-10-16(11-1
InchiKey:	RLLPVAHGXHCWKJ-IEBWSBKVSA-N
Formula:	C21H20Cl2O3
SMILES:	CC1(C)C(C=C(Cl)Cl)C1C(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	391.29
CAS:	61949-76-6

Physical Properties

Property code	Value	Unit	Source
gf	89.86	kJ/mol	Joback Method
hf	-268.89	kJ/mol	Joback Method
hfus	43.08	kJ/mol	Joback Method
hvap	86.07	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	6.113		Crippen Method
mcvol	281.860	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	913.47	K	Joback Method
tc	1160.83	K	Joback Method
tf	560.34	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.28	J/mol×K	1119.60	Joback Method
cpg	837.42	J/mol×K	913.47	Joback Method

cpg	855.30	J/mol×K	954.70	Joback Method
cpg	872.99	J/mol×K	995.92	Joback Method
cpg	890.73	J/mol×K	1037.15	Joback Method
cpg	908.75	J/mol×K	1078.38	Joback Method
cpg	946.56	J/mol×K	1160.83	Joback Method
hsubt	108.80	kJ/mol	323.00	NIST Webbook

Sources

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=C61949766&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hsubt:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume