Oxiranecarboxylic acid, 3-methyl-3-phenyl-, ethyl ester

Other names: Hydrocinnamic acid, «alpha»,«beta»-epoxy-«beta»-methyl-, ethyl ester
«alpha»,«beta»-Epoxy-«beta»-methylhydrocinnamic acid, ethyl ester
Ethyl «alpha»,«beta»-epoxy-«beta»-methylhydrocinnamate
Ethyl methylphenylglycidate
Fraeseol
3-Methyl-3-phenylglycidic acid ethyl ester
Ethyl «beta»-methyl-«beta»-phenylglycidate
Ethyl ester of 2,3-epoxy-3-phenylbutanoic acid
Ethyl 2,3-epoxy-3-methyl-3-phenylpropionate
EMPG
2,3-Epoxy-3-phenylbutyric acid, ethyl ester
Glycidic acid, 3-methyl-3-phenyl, ethyl ester
2-Oxiranecarboxylic acid, 3-methyl-3-phenyl-, ethyl ester
Aldehyde C-16
Ethyl 3-methyl-3-phenylglycidate
NSC 27905
Strawberry aldehyde
ethyl 2,3-epoxy-3-phenylbutyrate

Inchi: InChI=1S/C12H14O3/c1-3-14-11(13)10-12(2,15-10)9-7-5-4-6-8-9/h4-8,10H,3H2,1-2H3

InchiKey: LQKRYVGRPXFFAV-UHFFFAOYSA-N

Formula: C12H14O3

SMILES: CCOC(=O)C1OC1(C)c1ccccc1

Mol. weight [g/mol]: 206.24

CAS: 77-83-8

Physical Properties

Property code	Value	Unit	Source
gf	-109.92	kJ/mol	Joback Method
hf	-363.58	kJ/mol	Joback Method
hfus	24.55	kJ/mol	Joback Method
hvap	56.70	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.864		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook

tb	606.19	K	Joback Method
tc	833.43	K	Joback Method
tf	387.75	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.72	J/mol×K	606.19	Joback Method
cpg	424.92	J/mol×K	644.06	Joback Method
cpg	439.15	J/mol×K	681.94	Joback Method
cpg	452.55	J/mol×K	719.81	Joback Method
cpg	465.29	J/mol×K	757.68	Joback Method
cpg	477.50	J/mol×K	795.55	Joback Method
cpg	489.34	J/mol×K	833.43	Joback Method

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=C77838&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
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