

Oxiranecarboxylic acid, 3-phenyl-, ethyl ester

Other names:	Glycidic acid, 3-phenyl-, ethyl ester Ethyl «alpha»,«beta»-epoxyhydrocinnamate Ethyl phenylglycidate Ethyl 2,3-epoxy-3-phenylpropionate Ethyl 3-phenylglycidate Ethyl «alpha»,«beta»-epoxy-«alpha»-phenylpropionate ethyl 3-phenyloxirane-2-carboxylate
Inchi:	InChI=1S/C11H12O3/c1-2-13-11(12)10-9(14-10)8-6-4-3-5-7-8/h3-7,9-10H,2H2,1H3
InchiKey:	GOMAKLPNAAZVCJ-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	CCOC(=O)C1OC1c1ccccc1
Mol. weight [g/mol]:	192.21
CAS:	121-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-112.85	kJ/mol	Joback Method
hf	-358.18	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	55.63	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.690		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
tb	583.07	K	Joback Method
tc	805.72	K	Joback Method
tf	352.58	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.34	J/mol×K	583.07	Joback Method
cpg	428.43	J/mol×K	768.62	Joback Method
cpg	417.22	J/mol×K	731.51	Joback Method
cpg	405.15	J/mol×K	694.40	Joback Method
cpg	392.17	J/mol×K	657.29	Joback Method
cpg	378.25	J/mol×K	620.18	Joback Method
cpg	438.84	J/mol×K	805.72	Joback Method
dvisc	0.0005162	Pa×s	583.07	Joback Method
dvisc	0.0005976	Pa×s	544.65	Joback Method
dvisc	0.0007075	Pa×s	506.24	Joback Method
dvisc	0.0008611	Pa×s	467.82	Joback Method
dvisc	0.0010855	Pa×s	429.41	Joback Method
dvisc	0.0014322	Pa×s	391.00	Joback Method
dvisc	0.0020072	Pa×s	352.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	0.07	NIST Webbook

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=C121391&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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