

# Oxirane, [[4-(1,1-dimethylethyl)phenoxy]methyl]-

Other names:

p-tert-Butylphenyl glycidyl ether  
[[4-(1,1-Dimethylethyl)phenoxy]methyl]oxirane  
4-tert-Butylphenyl 2,3-epoxypropyl ether  
4-t-Butylphenyl glycidyl ether  
Propane, 1-(p-tert-butylphenoxy)-2,3-epoxy-  
tert-Butylphenol glycidyl ether  
3-(p-tert-Butylphenoxy)-1,2-epoxypropane  
tert-Butylphenyl glycidyl ether  
R 1007  
Heloxy 65  
Oxirane, 2-[[4-(1,1-dimethylethyl)phenoxy]methyl]-  
p-tert-butylphenyl 1-(2,3-epoxy)propyl ether

**Inchi:** InChI=1S/C13H18O2/c1-13(2,3)10-4-6-11(7-5-10)14-8-12-9-15-12/h4-7,12H,8-9H2,1-3H

**InchiKey:** HHRACYLRBOUBKM-UHFFFAOYSA-N

**Formula:** C13H18O2

**SMILES:** CC(C)(C)c1ccc(OCC2CO2)cc1

**Mol. weight [g/mol]:** 206.28

**CAS:** 3101-60-8

## Physical Properties

Property code	Value	Unit	Source
gf	33.83	kJ/mol	Joback Method
hf	-286.76	kJ/mol	Joback Method
hfus	22.97	kJ/mol	Joback Method
hvap	53.01	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.762		Crippen Method
mcvol	171.150	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
tb	581.38	K	Joback Method
tc	802.85	K	Joback Method
tf	344.37	K	Joback Method
vc	0.640	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.06	J/molxK	581.38	Joback Method
cpg	520.23	J/molxK	765.94	Joback Method
cpg	506.74	J/molxK	729.03	Joback Method
cpg	492.24	J/molxK	692.11	Joback Method
cpg	476.68	J/molxK	655.20	Joback Method
cpg	459.98	J/molxK	618.29	Joback Method
cpg	532.82	J/molxK	802.85	Joback Method
dvisc	0.0003171	Paxs	581.38	Joback Method
dvisc	0.0003871	Paxs	541.88	Joback Method
dvisc	0.0004876	Paxs	502.38	Joback Method
dvisc	0.0006388	Paxs	462.88	Joback Method
dvisc	0.0008802	Paxs	423.37	Joback Method
dvisc	0.0012955	Paxs	383.87	Joback Method
dvisc	0.0020837	Paxs	344.37	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.70	K	1.90	NIST Webbook

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method:

[https://en.wikipedia.org/wiki/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=C3101608&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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