

«alpha»-Methyl-«alpha»-[4-methyl-3-pentenyl]oxirane

Other names:	1,2-Oxolinalool
Inchi:	InChI=1S/C10H18O2/c1-8(2)5-4-6-10(3,11)9-7-12-9/h5,9,11H,4,6-7H2,1-3H3
InchiKey:	BXOURKNXQXLKRK-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CC(C)=CCCC(C)(O)C1CO1
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
hfus	23.34	kJ/mol	Joback Method
hvap	73.76	kJ/mol	Cheméo Relay (1.0)
log10ws	-1.44		Cheméo Relay (1.0)
logp	1.883		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
ripol	1446.00		NIST Webbook
tb	511.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.69	J/mol×K	554.88	Joback Method
cpg	396.66	J/mol×K	586.27	Joback Method
cpg	409.78	J/mol×K	617.66	Joback Method
cpg	422.09	J/mol×K	649.05	Joback Method
cpg	433.67	J/mol×K	680.45	Joback Method
cpg	444.58	J/mol×K	711.84	Joback Method
cpg	454.87	J/mol×K	743.23	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U132130&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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