

OXIRANECARBOXALDEHYDE, 3-METHYL-3-(4-METHYL-3-PENTENYL)-

Other names:	3-Methyl-3-(4-methylpent-3-en-1-yl)oxirane-2-carbaldehyde
Inchi:	InChI=1S/C10H16O2/c1-8(2)5-4-6-10(3)9(7-11)12-10/h5,7,9H,4,6H2,1-3H3
InchiKey:	KXDDDNKGVUBFQS-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CC(C)=CCCC1(C)OC1C=O
Mol. weight [g/mol]:	168.24

Physical Properties

Property code	Value	Unit	Source
hfus	23.72	kJ/mol	Joback Method
logp	2.089		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
rinpol	1236.20		NIST Webbook
rinpol	1236.20		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1215.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.52	J/mol×K	510.16	Joback Method
cpg	358.16		543.49	Joback Method
cpg	371.81	J/mol×K	576.82	Joback Method
cpg	384.59		610.15	Joback Method
cpg	396.62	J/mol×K	643.48	Joback Method
cpg	408.01		676.81	Joback Method
cpg	418.87	J/mol×K	710.14	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16996126&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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