

10-METHYLTRICYCLO[4.3.1.1(2,5)]UNDEC-3-EN-1

Other names:	10-Methyltricyclo[4.3.1.1(2,5)]undec-3-en-10-ol
Inchi:	InChI=1S/C12H18O/c1-12(13)10-3-2-4-11(12)9-6-5-8(10)7-9/h5-6,8-11,13H,2-4,7H2,1H3
InchiKey:	GCFBIUOSKKLHSD-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CC1(O)C2CCCC1C1C=CC2C1
Mol. weight [g/mol]:	178.28

Physical Properties

Property code	Value	Unit	Source
hfus	18.20	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.73	eV	NIST Webbook
logp	2.360		Crippen Method
mcvol	148.930	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.78	J/mol×K	584.96	Joback Method
cpg	438.42	J/mol×K	620.00	Joback Method
cpg	454.91	J/mol×K	655.03	Joback Method
cpg	470.39	J/mol×K	690.07	Joback Method
cpg	485.04	J/mol×K	725.10	Joback Method
cpg	499.01	J/mol×K	760.14	Joback Method
cpg	512.46	J/mol×K	795.17	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70220961&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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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