

1-CYCLOHEXENE-1-ETHANOL, 2,6,6-TRIMETHYL-

Other names:	«beta»-Cyclohomogeraniol
Inchi:	InChI=1S/C11H20O/c1-9-5-4-7-11(2,3)10(9)6-8-12/h12H,4-8H2,1-3H3
InchiKey:	JGJFZOVBGGQGOM-UHFFFAOYSA-N
Formula:	C11H20O
SMILES:	CC1=C(CCO)C(C)(C)CCC1
Mol. weight [g/mol]:	168.28

Physical Properties

Property code	Value	Unit	Source
hfus	14.31	kJ/mol	Joback Method
logp	2.895		Crippen Method
mcvol	156.560	ml/mol	McGowan Method
rinpol	1336.60		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.74	J/mol×K	572.17	Joback Method
cpg	412.89	J/mol×K	604.58	Joback Method
cpg	427.28	J/mol×K	637.00	Joback Method
cpg	440.98	J/mol×K	669.41	Joback Method
cpg	454.09	J/mol×K	701.83	Joback Method
cpg	466.68	J/mol×K	734.24	Joback Method
cpg	478.83	J/mol×K	766.66	Joback Method

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C472651&Units=SI>

Legend

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

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