

1,7-Octadiene, 2-methyl-6-methylene-

Other names:	«alpha»-Myrcene Alpha myrcene
Inchi:	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5H,1-2,4,6-8H2,3H3
InchiKey:	VYBREYK SZAROCT-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	<chem>C=CC(=C)CCCC(=C)C</chem>
Mol. weight [g/mol]:	136.23
CAS:	1686-30-2

Physical Properties

Property code	Value	Unit	Source
gf	279.74	kJ/mol	Joback Method
hf	106.98	kJ/mol	Joback Method
hfus	15.20	kJ/mol	Joback Method
hvap	36.00	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinpol	986.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	986.00		NIST Webbook
tb	418.00	K	Joback Method
tc	596.99	K	Joback Method
tf	169.26	K	Joback Method
vc	0.540	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.23	J/mol×K	418.00	Joback Method
cpg	281.30	J/mol×K	447.83	Joback Method
cpg	294.71	J/mol×K	477.66	Joback Method

cpg	307.48	J/mol×K	507.49	Joback Method
cpg	319.63	J/mol×K	537.32	Joback Method
cpg	331.20	J/mol×K	567.15	Joback Method
cpg	342.21	J/mol×K	596.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1686302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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