

«beta»-Myrcene

Other names:	.beta.-myrcene 1,6-Octadiene, 7-methyl-3-methylene- 2-Methyl-6-methylene-2,7-octadiene 3-Methylene-7-methyl-1,6-octadiene 7-Methyl-3-methylene-1,6-octadiene 7-Methyl-3-methyleneocta-1,6-diene 7-Methyl-3-methyleneoctadiene-(1,6) 7-methyl-3-methylene-1,6-octadiene (myrcene) 7-methyl-3-methylene-1,6-octadiene («beta»-myrcene) 7-methyl-3-methylene-1,6-octadiene (Â«betaÂ»-myrcene) Myrcene Myrcene, «beta»- Myrcene, Â«betaÂ»- NSC 406264 b-myrcene beta-Myrcene «beta»-Geraniolene «beta»-mircene Â«betaÂ»-Geraniolene Â«betaÂ»-mircene
Inchi:	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5,7H,1,4,6,8H2,2-3H3
InchiKey:	UAHWPYUMFXFJY-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	C=CC(=C)CCC=C(C)C
Mol. weight [g/mol]:	136.23
CAS:	123-35-3

Physical Properties

Property code	Value	Unit	Source
chl	-6236.30 ± 2.10	kJ/mol	NIST Webbook
gf	272.12	kJ/mol	Joback Method
hf	98.77	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	50.60	kJ/mol	NIST Webbook
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method
mcvol	138.860	ml/mol	McGowan Method

pc	2421.88	kPa	Joback Method
rinpol	991.00		NIST Webbook
rinpol	983.00		NIST Webbook
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ripol	1174.00		NIST Webbook
tb	440.20	K	NIST Webbook
tb	445.00 ± 5.00	K	NIST Webbook
tc	609.58	K	Joback Method
tf	165.94	K	Joback Method
vc	0.539	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	309.00	J/mol×K	517.53	Joback Method
cpg	321.31	J/mol×K	548.21	Joback Method
cpg	332.99	J/mol×K	578.90	Joback Method
cpg	267.94	J/mol×K	425.48	Joback Method
cpg	282.35	J/mol×K	456.16	Joback Method
cpg	296.03	J/mol×K	486.85	Joback Method
cpg	344.07	J/mol×K	609.58	Joback Method
hvapt	49.90	kJ/mol	298.15	Vapor pressure and vaporization enthalpy studies of (+)-longifolene, (-)-isolongifolene and beta-myrcene by correlation gas chromatography
hvapt	45.70	kJ/mol	366.00	NIST Webbook
hvapt	47.00	kJ/mol	333.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40858e+01
Coeff. B	-4.07501e+03
Coeff. C	-2.82800e+01
Temperature range (K), min.	282.55
Temperature range (K), max.	492.70

Sources

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The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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Vapour liquid equilibrium for -myrcene and carbon dioxide and/or hydrogen	https://www.doi.org/10.1016/j.fluid.2009.04.020
Vapor pressure and vaporization enthalpy studies of (+)-longifolene, (-)-isolongifolene and beta-myrcene by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2018.12.013
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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