«beta»-Ocimene

Other names:	1,3,6-Octatriene, 3,7-dimethyl- 3,7-Dimethyl-1,3,6-octatriene 3,7-dimethylocta-1,3,6-triene Ocimene beta-Ocimene
Inchi:	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5,7-8H,1,6H2,2-4H3
InchiKey:	IHPKGUQCSIINRJ-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	C=CC(C)=CCC=C(C)C
Mol. weight [g/mol]:	136.23
CAS:	13877-91-3

Physical Properties

Property code	Value	Unit	Source
gf	264.50	kJ/mol	Joback Method
hf	90.56	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	37.26	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	1037.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1044.00		NIST Webbook

rinpol	1035.00	NIST Webbook
rinpol	1037.00	NIST Webbook
rinpol	1037.00	NIST Webbook
rinpol	1035.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1023.00	NIST Webbook
rinpol	1026.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1031.00	NIST Webbook
rinpol	1027.60	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1041.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1024.00	NIST Webbook
rinpol	1031.00	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1037.00	NIST Webbook
rinpol	1048.00	NIST Webbook
ripol	1230.00	NIST Webbook
ripol	1235.00	NIST Webbook
ripol	1254.00	NIST Webbook
ripol	1259.00	NIST Webbook
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ripol	1259.00	NIST Webbook
ripol	1255.00	NIST Webbook
ripol	1247.00	NIST Webbook
ripol	1250.00	NIST Webbook
ripol	1250.00	NIST Webbook
ripol	1229.00	NIST Webbook
ripol	1254.00	NIST Webbook
ripol	1235.00	NIST Webbook
ripol	1230.00	NIST Webbook
ripol	1251.00	NIST Webbook
ripol	1247.00	NIST Webbook
ripol	1276.00	NIST Webbook
ripol	1233.00	NIST Webbook
ripol	1239.00	NIST Webbook
ripol	1252.00	NIST Webbook

ripol	1246.00		NIST Webbook
tb	432.96	K	Joback Method
tc	622.27	K	Joback Method
tf	162.62	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.68	J/mol×K	432.96	Joback Method
cpg	283.41	J/mol×K	464.51	Joback Method
cpg	297.33	J/mol×K	496.06	Joback Method
cpg	310.50	J/mol×K	527.62	Joback Method
cpg	322.94	J/mol×K	559.17	Joback Method
cpg	334.71	J/mol×K	590.72	Joback Method
cpg	345.84	J/mol×K	622.27	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59500e+01
Coeff. B	-4.35313e+03
Coeff. C	-6.95440e+01
Temperature range (K), min.	347.48
Temperature range (K), max.	478.73

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13877913&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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