1,3,7-Octatriene, 3,7-dimethyl-

Other names:	(3E)-3,7-Dimethyl-1,3,7-octatriene
	1,3,7-Octatrienene,3,7-dimethyl-
	2,6-Dimethyl-1,5,7-octatriene
	3,7-Dimethyl-1,3,7-octatriene
	3,7-Dimethylocta-1,3,7-triene
	Ocimene
	alpha-Ocimene
	«alpha»-Ocimene
	Â«alphaÂ»-Ocimene
Inchi:	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5,8H,1-2,6-7H2,3-4H3/b10-8+
InchiKey:	XJPBRODHZKDRCB-CSKARUKUSA-N
Formula:	C10H16
SMILES:	C=CC(C)=CCCC(=C)C
Mol. weight [g/mol]:	136.23
CAS:	502-99-8

Physical Properties

Property code	Value	Unit	Source
gf	272.12	kJ/mol	Joback Method
hf	98.77	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	36.63	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1042.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1052.00		NIST Webbook

rinpol	1040.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1018.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1052.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1039.50	NIST Webbook
rinpol	1051.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1038.00	NIST Webbook
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rinpol	1041.00	NIST Webbook
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rinpol	1038.00		NIST Webbook
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rinpol	1050.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1052.00		NIST Webbook
ripol	1254.00		NIST Webbook
ripol	1245.00		NIST Webbook
ripol	1237.00		NIST Webbook
ripol	1259.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1239.00		NIST Webbook
tb	425.48	K	Joback Method
tc	609.58	K	Joback Method
tf	165.94	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	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	344.07	J/mol×K	609.58	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=C502998&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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