

2,4,6-Octatriene, 2,6-dimethyl-

Other names:	Allo-Ocimene 2,6-Dimethyl-2,4,6-octatriene cis-Allo-ocimene Ocimene, A110 Neo-allo-ocimene Ocimene, allo- 2,6-dimethyl-octa-2,4,6-triene NSC 406263 (Z)-Alloocimene neo-allo-3,7-dimethyl-1,3,6-octatriene (neo-allo-ocimene) allo-3,7-dimethyl-1,3,6-octatriene (allo-ocimene)
Inchi:	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5-8H,1-4H3/b8-6+,10-5+
InchiKey:	GQVMHMFVBWSSPF-SOYUKNQ TSA-N
Formula:	C10H16
SMILES:	CC=C(C)C=CC=C(C)C
Mol. weight [g/mol]:	136.23
CAS:	673-84-7

Physical Properties

Property code	Value	Unit	Source
chl	-6197.80 ± 5.00	kJ/mol	NIST Webbook
gf	256.88	kJ/mol	Joback Method
hf	82.35	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	37.89	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1111.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1129.00		NIST Webbook
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ripol	1379.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1380.20		NIST Webbook
tb	440.44	K	Joback Method
tc	635.07	K	Joback Method
tf	247.51 ± 0.15	K	NIST Webbook
vc	0.537	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.43	J/mol×K	440.44	Joback Method
cpg	284.46	J/mol×K	472.88	Joback Method
cpg	298.62	J/mol×K	505.32	Joback Method
cpg	311.96	J/mol×K	537.75	Joback Method
cpg	324.52	J/mol×K	570.19	Joback Method
cpg	336.36	J/mol×K	602.63	Joback Method
cpg	347.53	J/mol×K	635.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C673847&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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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