allo- neo-Ocimene

Other names:	(E,E)-alloocimene
	2,6-Dimethyl-octa-2,4,6-triene, trans
	trans,trans-Alloocimene
	Alloocimene, trans
	4-trans-6-trans-alloocimene
	(E,E)-2,6-dimethylocta-2,4,6-triene
	2,4,6-Octatriene, 2,6-dimethyl-, (E,E)-
Inchi:	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5-8H,1-4H3/b8-6+,10-5+
InchiKey:	GQVMHMFBVWSSPF-SOYUKNQTSA-N
Formula:	C10H16
SMILES:	CC=C(C)C=CC=C(C)C
Mol. weight [g/mol]:	136.23
CAS:	3016-19-1

Physical Properties

Property code	Value	Unit	Source
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	1129.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1143.50		NIST Webbook
rinpol	1143.50		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1121.00		NIST Webbook
ripol	1393.00		NIST Webbook

ripol	1391.00		NIST Webbook
ripol	1393.00		NIST Webbook
ripol	1366.00		NIST Webbook
tb	440.44	K	Joback Method
tc	635.07	K	Joback Method
tf	159.30	K	Joback Method
vc	0.537	m3/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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.20	K	1.90	NIST Webbook

Sources

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=C3016191&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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