

2,4,6-Octatriene, 3,4-dimethyl-

Other names:	3,4-Dimethyl-2,4,6-octatriene
Inchi:	InChI=1S/C10H16/c1-5-7-8-10(4)9(3)6-2/h5-8H,1-4H3/b7-5+,9-6+,10-8+
InchiKey:	WGAUMWNVHAMGJF-AGPUZOHGSA-N
Formula:	C10H16
SMILES:	CC=CC=C(C)C(C)=CC
Mol. weight [g/mol]:	136.23
CAS:	57396-75-5

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	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1110.00		NIST Webbook
tb	440.44	K	Joback Method
tc	635.07	K	Joback Method
tf	159.30	K	Joback Method
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57396755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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