2,4,6-Octatriene, 2,6-dimethyl-, (E,Z)-

Other names:	(4E,6Z)-2,6-Dimethyl-2,4,6-octatriene
	(4E,6Z)-allo-Ocimene
	Neo-allo-ocimene
	(E,Z)-2,6-Dimethylocta-2,4,6-triene
	4-trans,6-cis-Allocimene
	Z-Neo-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:	GQVMHMFBVWSSPF-DAIHKBMKSA-N
Formula:	C10H16
SMILES:	CC=C(C)C=CC=C(C)C
Mol. weight [g/mol]:	136.23
CAS:	7216-56-0

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	1131.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1131.00		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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7216560&Units=SI
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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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