

2,6-Dimethyl-2-trans-6-octadiene

Other names:	trans-2,6-Dimethyl-2-6-octadiene 2,6-Dimethyl 2,6-octadiene (trans) trans-2,6-dimethyl-octa-2,6-diene 2,6-Dimethyl 2,6-octadiene (cis)
Inchi:	InChI=1S/C10H18/c1-5-10(4)8-6-7-9(2)3/h5,7H,6,8H2,1-4H3/b10-5+
InchiKey:	MZPDTOMKQCMETI-BJMVGYQFSA-N
Formula:	C10H18
SMILES:	CC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	138.25
CAS:	2609-23-6

Physical Properties

Property code	Value	Unit	Source
gf	176.66	kJ/mol	Joback Method
hf	-34.87	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	37.93	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.699		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	978.40		NIST Webbook
rinpol	1004.00		NIST Webbook
tb	436.28	K	Joback Method
tc	621.64	K	Joback Method
tf	164.38	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.91	J/mol×K	436.28	Joback Method
cpg	300.18	J/mol×K	467.17	Joback Method
cpg	314.68	J/mol×K	498.07	Joback Method

cpg	328.46	J/mol×K	528.96	Joback Method
cpg	341.53	J/mol×K	559.86	Joback Method
cpg	353.94	J/mol×K	590.75	Joback Method
cpg	365.73	J/mol×K	621.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2492220&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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