

1,3,6-Heptatriene, 2,5,5-trimethyl-

Other names:	2,5,5-Trimethyl-1,3,6-heptatriene 3,3,6-Trimethyl-1,4,6-heptatriene Artemisia triene
Inchi:	InChI=1S/C10H16/c1-6-10(4,5)8-7-9(2)3/h6-8H,1-2H2,3-5H3/b8-7+
InchiKey:	BYLJEQIUOXOYKOB-BQYQJAHWSA-N
Formula:	C10H16
SMILES:	<chem>C=CC(C)(C)C=CC(=C)C</chem>
Mol. weight [g/mol]:	136.23
CAS:	29548-02-5

Physical Properties

Property code	Value	Unit	Source
gf	283.51	kJ/mol	Joback Method
hf	99.81	kJ/mol	Joback Method
hfus	10.57	kJ/mol	Joback Method
hvap	35.26	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.331		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	918.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	921.00		NIST Webbook
ripol	1072.00		NIST Webbook
tb	422.37	K	Joback Method
tc	614.94	K	Joback Method
tf	182.32	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.89	J/mol×K	422.37	Joback Method
cpg	285.59	J/mol×K	454.47	Joback Method
cpg	300.33	J/mol×K	486.56	Joback Method
cpg	314.18	J/mol×K	518.66	Joback Method
cpg	327.17	J/mol×K	550.75	Joback Method
cpg	339.36	J/mol×K	582.85	Joback Method
cpg	350.80	J/mol×K	614.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29548025&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
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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