1,5-Heptadiene, 3,3,6-trimethyl-

Other names:	2,5,5-Trimethyl-2,6-heptadien
	2,5,5-Trimethyl-2,6-heptadiene
	2,6-Heptadiene, 2,5,5-trimethyl-
Inchi:	InChI=1S/C10H18/c1-6-10(4,5)8-7-9(2)3/h6-7H,1,8H2,2-5H3
InchiKey:	HRAGAKKBZWYBSJ-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	C=CC(C)(C)CC=C(C)C
Mol. weight [g/mol]:	138.25
CAS:	35387-63-4

Physical Properties

Property code	Value	Unit	Source
gf	195.67	kJ/mol	Joback Method
hf	-25.62	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	35.93	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	422.90 ± 2.00	K	NIST Webbook
tb	422.00 ± 3.00	K	NIST Webbook
tc	614.17	K	Joback Method
tf	184.08	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.88	J/mol×K	425.69	Joback Method
cpg	302.10	J/mol×K	457.10	Joback Method
cpg	317.41	J/mol×K	488.52	Joback Method
cpg	331.85	J/mol×K	519.93	Joback Method
cpg	345.47	J/mol×K	551.34	Joback Method

cpg	358.31	J/mol×K	582.76	Joback Method
cpg	370.43	J/mol×K	614.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35387634&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume