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

Other names: 2,3,6-Trimethyl-1,5-heptadiene
Inchi: InChI=1S/C10H18/c1-8(2)6-7-10(5)9(3)4/h6,10H,3,7H2,1-2,4-5H3
InchiKey: CHGRWGYJOYKPSL-UHFFFAOYSA-N
Formula: C10H18
SMILES: C=C(C)C(C)CC=C(C)C
Mol. weight [g/mol]: 138.25
CAS: 33501-88-1

Physical Properties

Property code	Value	Unit	Source
gf	181.84	kJ/mol	Joback Method
hf	-31.94	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	36.91	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	1063.00		NIST Webbook
tb	428.36	K	Joback Method
tc	612.80	K	Joback Method
tf	152.70	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.95	J/mol×K	428.36	Joback Method
cpg	299.33	J/mol×K	459.10	Joback Method
cpg	313.96	J/mol×K	489.84	Joback Method
cpg	327.88	J/mol×K	520.58	Joback Method
cpg	341.12	J/mol×K	551.32	Joback Method
cpg	353.71	J/mol×K	582.06	Joback Method
cpg	365.68	J/mol×K	612.80	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33501881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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