3-Hexene, 2,2,5,5-tetramethyl-

Other names: 2,2,5,5-tetramethylhex-3-ene
Inchi: InChI=1S/C10H20/c1-9(2,3)7-8-10(4,5)6/h7-8H,1-6H3
InchiKey: UYWLQEPMPVDASH-UHFFFAOYSA-N
Formula: C10H20
SMILES: CC(C)(C)C=CC(C)(C)C
Mol. weight [g/mol]: 140.27
CAS: 22808-06-6

Physical Properties

Property code	Value	Unit	Source
gf	119.22	kJ/mol	Joback Method
hf	-150.01	kJ/mol	Joback Method
hfus	7.03	kJ/mol	Joback Method
hvap	35.22	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.635		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
tb	398.40 ± 1.00	K	NIST Webbook
tb	396.40 ± 1.50	K	NIST Webbook
tb	398.16 ± 0.10	K	NIST Webbook
tc	618.91	K	Joback Method
tf	268.80 ± 1.00	K	NIST Webbook
tf	268.40 ± 0.10	K	NIST Webbook
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.07	J/mol×K	618.91	Joback Method
cpg	303.83	J/mol×K	425.90	Joback Method
cpg	321.95	J/mol×K	458.07	Joback Method
cpg	338.96	J/mol×K	490.24	Joback Method
cpg	354.91	J/mol×K	522.41	Joback Method

cpg	369.87	J/mol×K	554.58	Joback Method
cpg	383.91	J/mol×K	586.75	Joback Method
dvisc	0.0002185	Pa×s	425.90	Joback Method
dvisc	0.0185097	Pa×s	202.22	Joback Method
dvisc	0.0049656	Pa×s	239.50	Joback Method
dvisc	0.0018988	Pa×s	276.78	Joback Method
dvisc	0.0009122	Pa×s	314.06	Joback Method
dvisc	0.0005120	Pa×s	351.34	Joback Method
dvisc	0.0003211	Pa×s	388.62	Joback Method
hfust	10.25	kJ/mol	268.90	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22808066&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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

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