3,3,4-Trimethylpent-1-ene

Other names: 1-Pentene, 3,3,4-trimethyl-
3,3,4-trimethyl-1-pentene
Inchi: InChI=1S/C8H16/c1-6-8(4,5)7(2)3/h6-7H,1H2,2-5H3
InchiKey: LLFHCOGPDCJMKY-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=CC(C)(C)C(C)C
Mol. weight [g/mol]: 112.21
CAS: 560-22-5

Physical Properties

Property code	Value	Unit	Source
gf	104.72	kJ/mol	Joback Method
hf	-97.05	kJ/mol	Joback Method
hfus	4.26	kJ/mol	Joback Method
hvap	31.05	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.855		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	725.20		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	722.50		NIST Webbook
tb	378.60 ± 0.80	K	NIST Webbook
tb	378.00 ± 2.00	K	NIST Webbook
tc	557.61	K	Joback Method
tf	165.58	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.46	J/mol×K	375.45	Joback Method
cpg	284.07	J/mol×K	527.25	Joback Method
cpg	272.30	J/mol×K	496.89	Joback Method

cpg	259.89	J/mol×K	466.53	Joback Method
cpg	246.80	J/mol×K	436.17	Joback Method
cpg	233.00	J/mol×K	405.81	Joback Method
cpg	295.21	J/mol×K	557.61	Joback Method
dvisc	0.0002630	Pa×s	375.45	Joback Method
dvisc	0.0003729	Pa×s	340.47	Joback Method
dvisc	0.0005729	Pa×s	305.49	Joback Method
dvisc	0.0009836	Pa×s	270.51	Joback Method
dvisc	0.0019828	Pa×s	235.54	Joback Method
dvisc	0.0051039	Pa×s	200.56	Joback Method
dvisc	0.0195893	Pa×s	165.58	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C560225&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
KDB: https://www.cheric.org/files/research/kdb/mol/mol330.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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