2-Hexene, 3,5,5-trimethyl-

Other names:	3,5,5-Trimethyl-hex-2-ene
	3,5,5-Trimethyl-2-hexene
Inchi:	InChI=1S/C9H18/c1-6-8(2)7-9(3,4)5/h6H,7H2,1-5H3/b8-6+
InchiKey:	MXAFMRHRWMAVRM-SOFGYWHQSA-N
Formula:	C9H18
SMILES:	CC=C(C)CC(C)(C)C
Mol. weight [g/mol]:	126.24
CAS:	26456-76-8

Physical Properties

Property code	Value	Unit	Source
gf	99.41	kJ/mol	Joback Method
hf	-130.41	kJ/mol	Joback Method
hfus	10.54	kJ/mol	Joback Method
hvap	34.37	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	985.00		NIST Webbook
tb	433.70 ± 1.50	K	NIST Webbook
tb	435.00 ± 2.00	K	NIST Webbook
tc	592.11	K	Joback Method
tf	174.57	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.53	J/mol×K	406.13	Joback Method
cpg	275.34	J/mol×K	437.13	Joback Method
cpg	290.31	J/mol×K	468.12	Joback Method

cpg	304.47	J/mol×K	499.12	Joback Method
cpg	317.87	J/mol×K	530.11	Joback Method
cpg	330.54	J/mol×K	561.11	Joback Method
cpg	342.52	J/mol×K	592.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26456768&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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