2-Hexene, 2,4,4-trimethyl

Inchi: InChI=1S/C9H18/c1-6-9(4,5)7-8(2)3/h7H,6H2,1-5H3
InchiKey: WPYKNDOCNBOBHN-UHFFFAOYSA-N
Formula: C9H18
SMILES: CCC(C)(C)C=C(C)C
Mol. weight [g/mol]: 126.24

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	702.00		NIST Webbook
rinpol	702.00		NIST Webbook
tb	406.13	K	Joback Method
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

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=R569298&Units=SI

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