2,3,3-Trimethyl-1-hexene

Inchi: InChI=1S/C9H18/c1-6-7-9(4,5)8(2)3/h2,6-7H2,1,3-5H3
InchiKey: FJJUXGUOHOVYPK-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=C(C)C(C)(C)CCC
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	107.03	kJ/mol	Joback Method
hf	-122.20	kJ/mol	Joback Method
hfus	9.06	kJ/mol	Joback Method
hvap	33.74	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	824.00		NIST Webbook
rinpol	825.00		NIST Webbook
tb	398.65	K	Joback Method
tc	579.25	K	Joback Method
tf	177.89	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.60	J/mol×K	398.65	Joback Method
cpg	274.01	J/mol×K	428.75	Joback Method
cpg	288.67	J/mol×K	458.85	Joback Method
cpg	302.59	J/mol×K	488.95	Joback Method
cpg	315.80	J/mol×K	519.05	Joback Method
cpg	328.34	J/mol×K	549.15	Joback Method
cpg	340.24	J/mol×K	579.25	Joback Method

Sources

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=U113521&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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