

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
CAS:	700000-97-1

Physical Properties

Property code	Value	Unit	Source
af	0.2690		Cheméo Relay (1.0)
gf	107.03	kJ/mol	Joback Method
hf	-126.98	kJ/mol	Cheméo Relay (1.0)
hfus	9.06	kJ/mol	Joback Method
hvap	39.26	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
log10ws	-4.52		Cheméo Relay (1.0)
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
tb	404.90 ± 0.60	K	NIST Webbook
tc	578.34	K	Cheméo Relay (1.0)
tf	173.60 ± 2.00	K	NIST Webbook
vc	0.477	m3/kmol	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C700000971&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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