3,3-dimethyl-1-heptene

Inchi: InChI=1S/C9H18/c1-5-7-8-9(3,4)6-2/h6H,2,5,7-8H2,1,3-4H3
InchiKey: WETAFQBUDAJCAM-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=CC(C)(C)CCCC
Mol. weight [g/mol]: 126.24
CAS: 19549-89-4

Physical Properties

Property code	Value	Unit	Source
af	0.2982		Cheméo Relay (1.0)
gf	115.58	kJ/mol	Joback Method
hf	-121.21	kJ/mol	Cheméo Relay (1.0)
hfus	10.37	kJ/mol	Joback Method
hvap	38.73	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.67		Cheméo Relay (1.0)
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
tb	401.65	K	Cheméo Relay (1.0)
tc	567.41	K	Cheméo Relay (1.0)
tf	161.66	K	Cheméo Relay (1.0)
vc	0.486	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.63	J/mol×K	398.77	Joback Method
cpg	339.09	J/mol×K	575.86	Joback Method
cpg	327.33	J/mol×K	546.34	Joback Method
cpg	314.95	J/mol×K	516.83	Joback Method
cpg	301.92	J/mol×K	487.31	Joback Method
cpg	288.21	J/mol×K	457.80	Joback Method
cpg	273.79	J/mol×K	428.28	Joback Method
dvisc	0.0008443	Pa×s	295.31	Joback Method

dvisc	0.0002617	Pa×s	398.77	Joback Method
dvisc	0.0003591	Pa×s	364.28	Joback Method
dvisc	0.0005266	Pa×s	329.80	Joback Method
dvisc	0.0096355	Pa×s	191.85	Joback Method
dvisc	0.0015337	Pa×s	260.82	Joback Method
dvisc	0.0033420	Pa×s	226.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52155e+01
Coeff. B	-3.82274e+03
Coeff. C	-5.68400e+01
Temperature range (K), min.	312.92
Temperature range (K), max.	442.82

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19549894&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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume