4,5-dimethyl-2-heptene

Inchi: InChI=1S/C9H18/c1-5-7-9(4)8(3)6-2/h5,7-9H,6H2,1-4H3/b7-5+
InchiKey: HXSUSWIKNRAROU-FNORWQNLSA-N
Formula: C9H18
SMILES: CC=CC(C)C(C)CC
Mol. weight [g/mol]: 126.24
CAS: ---

Physical Properties

Property code	Value	Unit	Source
gf	100.24	kJ/mol	Joback Method
hf	-122.43	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	34.81	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.245		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	837.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	837.00		NIST Webbook
tb	408.60	K	Joback Method
tc	587.67	K	Joback Method
tf	156.11	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.97	J/mol×K	408.60	Joback Method
cpg	272.79	J/mol×K	438.45	Joback Method
cpg	286.94	J/mol×K	468.29	Joback Method
cpg	300.46	J/mol×K	498.14	Joback Method
cpg	313.37	J/mol×K	527.98	Joback Method
cpg	325.70	J/mol×K	557.83	Joback Method

cpg	337.45	J/mol×K	587.67	Joback Method
dvisc	0.0223846	Pa×s	156.11	Joback Method
dvisc	0.0043187	Pa×s	198.19	Joback Method
dvisc	0.0014827	Pa×s	240.27	Joback Method
dvisc	0.0007001	Pa×s	282.36	Joback Method
dvisc	0.0004016	Pa×s	324.44	Joback Method
dvisc	0.0002618	Pa×s	366.52	Joback Method
dvisc	0.0001863	Pa×s	408.60	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

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=R141370&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume