3,5-Dimethyl-1-hexene

Other names: 3,5-Dimethylhex-1-ene
Inchi: InChI=1S/C8H16/c1-5-8(4)6-7(2)3/h5,7-8H,1,6H2,2-4H3
InchiKey: FEZKAPRRVNNJTK-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=CC(C)CC(C)C
Mol. weight [g/mol]: 112.22
CAS: 7423-69-0

Physical Properties

Property code	Value	Unit	Source
af	0.2850		Cheméo Relay (1.0)
gf	99.44	kJ/mol	Joback Method
hf	-106.52	kJ/mol	Cheméo Relay (1.0)
hfus	8.15	kJ/mol	Joback Method
hvap	38.10	kJ/mol	NIST Webbook
ie	9.43	eV	Cheméo Relay (1.0)
log10ws	-4.25		Cheméo Relay (1.0)
logp	2.855		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	718.01		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	699.50		NIST Webbook
tb	375.52	K	Cheméo Relay (1.0)
tc	527.13	K	Cheméo Relay (1.0)
tf	154.95	K	Cheméo Relay (1.0)
vc	0.428	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.47	J/mol×K	378.24	Joback Method
cpg	230.74	J/mol×K	407.35	Joback Method

cpg	243.47	J/mol×K	436.46	Joback Method
cpg	255.68	J/mol×K	465.57	Joback Method
cpg	267.38	J/mol×K	494.69	Joback Method
cpg	278.59	J/mol×K	523.80	Joback Method
cpg	289.32	J/mol×K	552.91	Joback Method
dvisc	0.0184203	Pa×s	148.16	Joback Method
dvisc	0.0041486	Pa×s	186.51	Joback Method
dvisc	0.0015535	Pa×s	224.85	Joback Method
dvisc	0.0007745	Pa×s	263.20	Joback Method
dvisc	0.0004609	Pa×s	301.55	Joback Method
dvisc	0.0003084	Pa×s	339.89	Joback Method
dvisc	0.0002238	Pa×s	378.24	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.26083e+01
Coeff. B	-2.67112e+03
Coeff. C	-5.90470e+01
Temperature range (K), min.	275.85
Temperature range (K), max.	425.11

Sources

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):

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=C7423690&Units=SI

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
ie:	Ionization energy
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