

1-Heptene, 6-methyl-

Other names:	6-Methyl-1-heptene 6-Methylhept-1-ene
Inchi:	InChI=1S/C8H16/c1-4-5-6-7-8(2)3/h4,8H,1,5-7H2,2-3H3
InchiKey:	DFVOXRAAHOJJBN-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	C=CCCCC(C)C
Mol. weight [g/mol]:	112.21
CAS:	5026-76-6

Physical Properties

Property code	Value	Unit	Source
gf	101.88	kJ/mol	Joback Method
hf	-88.30	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	38.90	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	753.00		NIST Webbook
rinpol	754.40		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	754.40		NIST Webbook
rinpol	746.20		NIST Webbook
rinpol	742.50		NIST Webbook
rinpol	749.40		NIST Webbook
rinpol	749.40		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	748.00		NIST Webbook
tb	387.15 ± 3.00	K	NIST Webbook
tb	384.65 ± 2.00	K	NIST Webbook
tb	386.60 ± 0.50	K	NIST Webbook
tb	386.15 ± 2.00	K	NIST Webbook

tb	384.65 ± 0.60	K	NIST Webbook
tb	385.80 ± 1.00	K	NIST Webbook
tb	386.35 ± 0.20	K	NIST Webbook
tb	386.34 ± 0.20	K	NIST Webbook
tb	386.34 ± 0.20	K	NIST Webbook
tb	386.34 ± 0.20	K	NIST Webbook
tb	386.34 ± 0.20	K	NIST Webbook
tb	386.34 ± 0.40	K	NIST Webbook
tb	388.65 ± 2.00	K	NIST Webbook
tb	402.15 ± 3.00	K	NIST Webbook
tc	549.32	K	Joback Method
tf	163.16	K	Joback Method
vc	0.459	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.60	J/mol×K	378.68	Joback Method
cpg	277.03	J/mol×K	520.88	Joback Method
cpg	266.10	J/mol×K	492.44	Joback Method
cpg	254.71	J/mol×K	464.00	Joback Method
cpg	242.84	J/mol×K	435.56	Joback Method
cpg	230.47	J/mol×K	407.12	Joback Method
cpg	287.50	J/mol×K	549.32	Joback Method
dvisc	0.0002308	Paxs	378.68	Joback Method
dvisc	0.0003075	Paxs	342.76	Joback Method
dvisc	0.0004381	Paxs	306.84	Joback Method
dvisc	0.0006856	Paxs	270.92	Joback Method
dvisc	0.0012304	Paxs	235.00	Joback Method
dvisc	0.0027265	Paxs	199.08	Joback Method
dvisc	0.0085772	Paxs	163.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42264e+01

Coeff. B	-3.22125e+03
Coeff. C	-5.07340e+01
Temperature range (K), min.	281.83
Temperature range (K), max.	412.07

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5026766&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol260.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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