

2-Methyl-3-heptene

Inchi:	InChI=1S/C8H16/c1-4-5-6-7-8(2)3/h6-8H,4-5H2,1-3H3/b7-6+
InchiKey:	CYEZJYAMLNTSKN-VOTSOKGWSA-N
Formula:	C8H16
SMILES:	CCCC=CC(C)C
Mol. weight [g/mol]:	112.21
CAS:	17618-76-7

Physical Properties

Property code	Value	Unit	Source
gf	94.26	kJ/mol	Joback Method
hf	-96.51	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	32.97	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	759.00		NIST Webbook
rinpol	759.00		NIST Webbook
tb	386.16	K	Joback Method
tc	562.05	K	Joback Method
tf	159.84	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.94	J/molxK	386.16	Joback Method
cpg	231.23	J/molxK	415.47	Joback Method
cpg	243.94	J/molxK	444.79	Joback Method
cpg	256.10	J/molxK	474.10	Joback Method
cpg	267.72	J/molxK	503.42	Joback Method
cpg	278.83	J/molxK	532.73	Joback Method
cpg	289.43	J/molxK	562.05	Joback Method

dvisc	0.0101457	Paxs	159.84	Joback Method
dvisc	0.0028001	Paxs	197.56	Joback Method
dvisc	0.0011677	Paxs	235.28	Joback Method
dvisc	0.0006201	Paxs	273.00	Joback Method
dvisc	0.0003840	Paxs	310.72	Joback Method
dvisc	0.0002638	Paxs	348.44	Joback Method
dvisc	0.0001950	Paxs	386.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41614e+01
Coeff. B	-3.29361e+03
Coeff. C	-4.82220e+01
Temperature range (K), min.	285.62
Temperature range (K), max.	420.39

Sources

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=R593261&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

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

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