3-Methyl-2-hexene

Other names: 2-Hexene, 3-methyl
Inchi: InChI=1S/C7H14/c1-4-6-7(3)5-2/h5H,4,6H2,1-3H3
InchiKey: JZMUUSXQSKCZNO-UHFFFAOYSA-N
Formula: C7H14
SMILES: CC=C(C)CCC
Mol. weight [g/mol]: 98.19
CAS: 17618-77-8

Physical Properties

Property code	Value	Unit	Source
gf	79.73	kJ/mol	Joback Method
hf	-80.38	kJ/mol	Joback Method
hfus	12.78	kJ/mol	Joback Method
hvap	31.21	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	708.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	702.00		NIST Webbook
tb	361.00 ± 6.00	K	NIST Webbook
tb	368.00 ± 6.00	K	NIST Webbook
tb	365.15 ± 3.00	K	NIST Webbook
tb	369.40 ± 2.00	K	NIST Webbook
tb	367.55 ± 2.00	K	NIST Webbook
tb	368.15 ± 3.00	K	NIST Webbook
tb	366.35 ± 2.00	K	NIST Webbook
tc	539.41	K	Joback Method
tf	149.61	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.34	J/mol×K	363.60	Joback Method
cpg	192.22	J/mol×K	392.90	Joback Method
cpg	203.59	J/mol×K	422.20	Joback Method
cpg	214.47	J/mol×K	451.50	Joback Method
cpg	224.86	J/mol×K	480.80	Joback Method
cpg	234.79	J/mol×K	510.11	Joback Method
cpg	244.29	J/mol×K	539.41	Joback Method

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=C17618778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
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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