4-Methyl-2-heptene

Other names: 2-heptene, 4-methyl-
Inchi: InChI=1S/C8H16/c1-4-6-8(3)7-5-2/h4,6,8H,5,7H2,1-3H3
InchiKey: SVGLFIBXFVQUQY-UHFFFAOYSA-N
Formula: C8H16
SMILES: CC=CC(C)CCC
Mol. weight [g/mol]: 112.21
CAS: 3404-56-6

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	746.20		NIST Webbook
rinpol	746.20		NIST Webbook
tb	387.10 ± 0.60	K	NIST Webbook
tb	386.65 ± 0.50	K	NIST Webbook
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/mol×K	386.16	Joback Method
cpg	231.23	J/mol×K	415.47	Joback Method
cpg	243.94	J/mol×K	444.79	Joback Method
cpg	256.10	J/mol×K	474.10	Joback Method
cpg	267.72	J/mol×K	503.42	Joback Method

cpg	278.83	J/mol×K	532.73	Joback Method
cpg	289.43	J/mol×K	562.05	Joback Method
dvisc	0.0101457	Pa×s	159.84	Joback Method
dvisc	0.0028001	Pa×s	197.56	Joback Method
dvisc	0.0011677	Pa×s	235.28	Joback Method
dvisc	0.0006201	Pa×s	273.00	Joback Method
dvisc	0.0003840	Pa×s	310.72	Joback Method
dvisc	0.0002638	Pa×s	348.44	Joback Method
dvisc	0.0001950	Pa×s	386.16	Joback Method

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=C3404566&Units=SI

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