2-Methyl-2-octene

Other names: 2-Octene, 2-methyl
Inchi: InChI=1S/C9H18/c1-4-5-6-7-8-9(2)3/h8H,4-7H2,1-3H3
InchiKey: YBOZNTGUYASNRA-UHFFFAOYSA-N
Formula: C9H18
SMILES: CCCCCC=C(C)C
Mol. weight [g/mol]: 126.24
CAS: 16993-86-5

Physical Properties

Property code	Value	Unit	Source
gf	96.57	kJ/mol	Joback Method
hf	-121.66	kJ/mol	Joback Method
hfus	17.96	kJ/mol	Joback Method
hvap	35.67	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.533		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	881.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	876.00		NIST Webbook
tb	418.00 ± 15.00	K	NIST Webbook
tc	583.79	K	Joback Method
tf	172.15	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.03	J/mol×K	409.36	Joback Method
cpg	272.25	J/mol×K	438.43	Joback Method
cpg	285.86	J/mol×K	467.50	Joback Method
cpg	298.88	J/mol×K	496.58	Joback Method
cpg	311.33	J/mol×K	525.65	Joback Method
cpg	323.24	J/mol×K	554.72	Joback Method
cpg	334.62	J/mol×K	583.79	Joback Method

Sources

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=C16993865&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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