2,3-Dimethyl-2-heptene

Other names: 2-Heptene, 2,3-dimethyl-
n-C4H9C(CH3)=C(CH3)2
Inchi: InChI=1S/C9H18/c1-5-6-7-9(4)8(2)3/h5-7H2,1-4H3
InchiKey: PTUNZAOKLBTUBF-UHFFFAOYSA-N
Formula: C9H18
SMILES: CCCCC(C)=C(C)C
Mol. weight [g/mol]: 126.24
CAS: 3074-64-4

Physical Properties

Property code	Value	Unit	Source
gf	88.02	kJ/mol	Joback Method
hf	-131.45	kJ/mol	Joback Method
hfus	16.65	kJ/mol	Joback Method
hvap	35.75	kJ/mol	Joback Method
ie	8.14 ± 0.01	eV	NIST Webbook
log10ws	-3.44		Crippen Method
logp	3.533		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	877.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	876.00		NIST Webbook
tb	418.30 ± 0.40	K	NIST Webbook
tb	419.00 ± 2.00	K	NIST Webbook
tc	587.07	K	Joback Method
tf	164.70 ± 2.00	K	NIST Webbook
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.99	J/mol×K	409.24	Joback Method
cpg	272.45	J/mol×K	438.88	Joback Method
cpg	286.28	J/mol×K	468.52	Joback Method
cpg	299.49	J/mol×K	498.15	Joback Method
cpg	312.12	J/mol×K	527.79	Joback Method
cpg	324.18	J/mol×K	557.43	Joback Method
cpg	335.71	J/mol×K	587.07	Joback Method

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol343.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3074644&Units=SI
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

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
ie: Ionization energy
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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