1-Heptene, 2,6-dimethyl-

Other names: 2,6-Dimethyl-1-heptene
Inchi: InChI=1S/C9H18/c1-8(2)6-5-7-9(3)4/h9H,1,5-7H2,2-4H3
InchiKey: JUUMAEXLYIMEOD-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=C(C)CCCC(C)C
Mol. weight [g/mol]: 126.24
CAS: 3074-78-0

Physical Properties

Property code	Value	Unit	Source
gf	101.75	kJ/mol	Joback Method
hf	-118.73	kJ/mol	Joback Method
hfus	12.95	kJ/mol	Joback Method
hvap	45.90 ± 0.50	kJ/mol	NIST Webbook
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	866.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	866.00		NIST Webbook
ripol	844.00		NIST Webbook
ripol	844.00		NIST Webbook
tb	415.00 ± 5.00	K	NIST Webbook
tc	574.80	K	Joback Method
tf	160.47	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.19	J/mol×K	401.44	Joback Method
cpg	271.44	J/mol×K	430.33	Joback Method
cpg	285.11	J/mol×K	459.23	Joback Method
cpg	298.22	J/mol×K	488.12	Joback Method
cpg	310.78	J/mol×K	517.01	Joback Method
cpg	322.81	J/mol×K	545.91	Joback Method
cpg	334.34	J/mol×K	574.80	Joback Method
hvapt	46.30 ± 0.50	kJ/mol	289.50	NIST Webbook

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=C3074780&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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume