2-Heptene, 2,6-dimethyl-

Other names: 2,6-Dimethyl-2-heptene
Inchi: InChI=1S/C9H18/c1-8(2)6-5-7-9(3)4/h6,9H,5,7H2,1-4H3
InchiKey: JDJYGSMZGYTCML-UHFFFAOYSA-N
Formula: C9H18
SMILES: CC(C)=CCCC(C)C
Mol. weight [g/mol]: 126.24
CAS: 5557-98-2

Physical Properties

Property code	Value	Unit	Source
gf	94.13	kJ/mol	Joback Method
hf	-126.94	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	35.28	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
tb	409.00 ± 3.00	K	NIST Webbook
tc	587.37	K	Joback Method
tf	157.15	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.98	J/mol×K	408.92	Joback Method
cpg	272.62	J/mol×K	438.66	Joback Method
cpg	286.61	J/mol×K	468.40	Joback Method
cpg	299.98	J/mol×K	498.14	Joback Method
cpg	312.75	J/mol×K	527.89	Joback Method

cpg	324.94	J/mol×K	557.63	Joback Method
cpg	336.58	J/mol×K	587.37	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=C5557982&Units=SI

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