2,4-Dimethyl-1-heptene

Other names: 1-Heptene, 2,4-dimethyl
Inchi: InChI=1S/C9H18/c1-5-6-9(4)7-8(2)3/h9H,2,5-7H2,1,3-4H3
InchiKey: CZGAOHSMVSIJJZ-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=C(C)CC(C)CCC
Mol. weight [g/mol]: 126.24
CAS: 19549-87-2

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	34.65	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	828.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	836.20		NIST Webbook
rinpol	836.20		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	844.00		NIST Webbook
ripol	885.00		NIST Webbook
tb	401.44	K	Joback Method
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

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=C19549872&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
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume