

Heptane, 2,2,3,3,5,6,6-heptamethyl-

Other names:	2,2,3,3,5,6,6-Heptamethylheptane
Inchi:	InChI=1S/C14H30/c1-11(12(2,3)4)10-14(8,9)13(5,6)7/h11H,10H2,1-9H3
InchiKey:	OTNCYIBPUVFLLZ-UHFFFAOYSA-N
Formula:	C14H30
SMILES:	CC(CC(C)(C)C(C)(C)C(C)(C)C
Mol. weight [g/mol]:	198.39
CAS:	7225-67-4

Physical Properties

Property code	Value	Unit	Source
gf	73.08	kJ/mol	Joback Method
hf	-363.82	kJ/mol	Joback Method
hfus	6.25	kJ/mol	Joback Method
hvap	42.48	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	5.131		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
tb	509.59	K	Joback Method
tc	701.25	K	Joback Method
tf	239.80	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.95	J/molxK	509.59	Joback Method
cpg	535.43	J/molxK	541.53	Joback Method
cpg	556.58	J/molxK	573.48	Joback Method
cpg	576.46	J/molxK	605.42	Joback Method
cpg	595.16	J/molxK	637.36	Joback Method
cpg	612.73	J/molxK	669.31	Joback Method
cpg	629.27	J/molxK	701.25	Joback Method
dvisc	0.0297494	Paxs	239.80	Joback Method

dvisc	0.0061737	Paxs	284.76	Joback Method
dvisc	0.0019673	Paxs	329.73	Joback Method
dvisc	0.0008249	Paxs	374.69	Joback Method
dvisc	0.0004167	Paxs	419.66	Joback Method
dvisc	0.0002402	Paxs	464.62	Joback Method
dvisc	0.0001526	Paxs	509.59	Joback Method

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=C7225674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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