

Heptane, 2,2,3,5-tetramethyl-

Inchi:	InChI=1S/C11H24/c1-7-9(2)8-10(3)11(4,5)6/h9-10H,7-8H2,1-6H3
InchiKey:	KXNFNEAZTWCHIL-UHFFFAOYSA-N
Formula:	C11H24
SMILES:	CCC(C)CC(C)C(C)(C)C
Mol. weight [g/mol]:	156.31
CAS:	61868-42-6

Physical Properties

Property code	Value	Unit	Source
gf	39.70	kJ/mol	Joback Method
hf	-289.68	kJ/mol	Joback Method
hfus	9.79	kJ/mol	Joback Method
hvap	38.01	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	4.105		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
tb	446.97	K	Joback Method
tc	625.99	K	Joback Method
tf	186.15	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.01	J/molxK	446.97	Joback Method
cpg	380.31	J/molxK	476.81	Joback Method
cpg	397.75	J/molxK	506.64	Joback Method
cpg	414.36	J/molxK	536.48	Joback Method
cpg	430.18	J/molxK	566.32	Joback Method
cpg	445.24	J/molxK	596.15	Joback Method
cpg	459.56	J/molxK	625.99	Joback Method
dvisc	0.0387426	Paxs	186.15	Joback Method
dvisc	0.0071443	Paxs	229.62	Joback Method

dvisc	0.0022567	Paxs	273.09	Joback Method
dvisc	0.0009782	Paxs	316.56	Joback Method
dvisc	0.0005189	Paxs	360.03	Joback Method
dvisc	0.0003155	Paxs	403.50	Joback Method
dvisc	0.0002114	Paxs	446.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C61868426&Units=SI

Legend

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

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