

Heptane, 2,2,6-trimethyl-

Other names:	2,2,6-Trimethylheptane
Inchi:	InChI=1S/C10H22/c1-9(2)7-6-8-10(3,4)5/h9H,6-8H2,1-5H3
InchiKey:	FHJCGIUZJXWNET-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CC(C)CCCC(C)(C)C
Mol. weight [g/mol]:	142.28
CAS:	1190-83-6

Physical Properties

Property code	Value	Unit	Source
gf	33.72	kJ/mol	Joback Method
hf	-263.76	kJ/mol	Joback Method
hfus	10.72	kJ/mol	Joback Method
hvap	46.40	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	872.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	873.00		NIST Webbook
tb	421.15 ± 3.00	K	NIST Webbook
tb	421.15 ± 3.00	K	NIST Webbook
tb	421.35 ± 1.50	K	NIST Webbook
tb	422.08 ± 0.40	K	NIST Webbook
tb	421.65 ± 3.00	K	NIST Webbook
tc	600.93	K	Joback Method
tf	168.15 ± 1.00	K	NIST Webbook
vc	0.579	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.93	J/molxK	424.53	Joback Method
cpg	333.94	J/molxK	453.93	Joback Method
cpg	350.18	J/molxK	483.33	Joback Method
cpg	365.66	J/molxK	512.73	Joback Method
cpg	380.41	J/molxK	542.13	Joback Method
cpg	394.47	J/molxK	571.53	Joback Method
cpg	407.85	J/molxK	600.93	Joback Method
dvisc	0.0206027	Paxs	189.88	Joback Method
dvisc	0.0052013	Paxs	228.99	Joback Method
dvisc	0.0019620	Paxs	268.10	Joback Method
dvisc	0.0009486	Paxs	307.20	Joback Method
dvisc	0.0005405	Paxs	346.31	Joback Method
dvisc	0.0003452	Paxs	385.42	Joback Method
dvisc	0.0002394	Paxs	424.53	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39245e+01
Coeff. B	-3.27889e+03
Coeff. C	-6.97560e+01
Temperature range (K), min.	310.20
Temperature range (K), max.	450.44

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1190836&Units=SI>

The Yaws Handbook of Vapor

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

**Pressure:
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

KDB: <https://www.cheric.org/files/research/kdb/mol/mol129.mol>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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