Heptane, 3,3,5-trimethyl-

Other names: 3,3,5-Trimethylheptane
Inchi: InChI=1S/C10H22/c1-6-9(3)8-10(4,5)7-2/h9H,6-8H2,1-5H3
InchiKey: VRVRZZWPKABUOE-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCC(C)CC(C)(C)CC
Mol. weight [g/mol]: 142.28
CAS: 7154-80-5

Physical Properties

Property code	Value	Unit	Source
af	0.3820		KDB
ap	343.150	K	KDB
gf	33.58	kJ/mol	KDB
hcg	6775.90	kJ/mol	KDB
hcn	6291.816	kJ/mol	KDB
hf	-258.70	kJ/mol	KDB
hfus	10.72	kJ/mol	Joback Method
hvap	46.00	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2320.00 ± 40.00	kPa	NIST Webbook
pc	2320.00	kPa	KDB
pc	2317.00 ± 20.00	kPa	NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	907.70		NIST Webbook
rinpol	907.70		NIST Webbook
rinpol	913.20		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	913.20		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	913.00		NIST Webbook

rinpol	913.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	913.00		NIST Webbook
tb	428.83 ± 0.30	K	NIST Webbook
tb	434.70 ± 1.50	K	NIST Webbook
tb	428.80 ± 0.30	K	NIST Webbook
tb	428.80	K	KDB
tc	609.50	K	KDB
tc	609.50 ± 0.50	K	NIST Webbook
tc	609.55 ± 0.15	K	NIST Webbook
tf	219.00	K	KDB
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.93	J/mol×K	424.53	Joback Method
cpg	333.94	J/mol×K	453.93	Joback Method
cpg	350.18	J/mol×K	483.33	Joback Method
cpg	365.66	J/mol×K	512.73	Joback Method
cpg	380.41	J/mol×K	542.13	Joback Method
cpg	394.47	J/mol×K	571.53	Joback Method
cpg	407.85	J/mol×K	600.93	Joback Method
dvisc	0.0052013	Pa×s	228.99	Joback Method
dvisc	0.0206027	Pa×s	189.88	Joback Method
dvisc	0.0019620	Pa×s	268.10	Joback Method
dvisc	0.0009486	Pa×s	307.20	Joback Method
dvisc	0.0005405	Pa×s	346.31	Joback Method
dvisc	0.0003452	Pa×s	385.42	Joback Method
dvisc	0.0002394	Pa×s	424.53	Joback Method
hvapt	36.65	kJ/mol	428.90	KDB
rfi	1.41470		298.15	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42396e+01
Coeff. B	-3.58051e+03
Coeff. C	-5.67030e+01
Temperature range (K), min.	313.33
Temperature range (K), max.	457.74

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.70461e+01
Coeff. B	-8.69026e+03
Coeff. C	-1.21313e+01
Coeff. D	7.43061e-06
Temperature range (K), min.	313.00
Temperature range (K), max.	609.50

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7154805&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=139

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=139

Legend

af: Acentric Factor

ap: Aniline Point

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hcg: Heat of Combustion, Gross form

hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume