Heptane, 3,4,5-trimethyl-

Other names: 3,4,5-Trimethylheptane
Inchi: InChI=1S/C10H22/c1-6-8(3)10(5)9(4)7-2/h8-10H,6-7H2,1-5H3
InchiKey: LJIIBBYARMPSMT-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCC(C)C(C)C(C)CC
Mol. weight [g/mol]: 142.28
CAS: 20278-89-1

Physical Properties

Property code	Value	Unit	Source
af	0.4170		KDB
gf	26.00	kJ/mol	Joback Method
hcg	6775.90	kJ/mol	KDB
hcn	6291.774	kJ/mol	KDB
hf	-265.57	kJ/mol	Joback Method
hfus	11.09	kJ/mol	Joback Method
hvap	47.30	kJ/mol	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.715		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2240.00	kPa	KDB
rinpol	945.90		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	945.20		NIST Webbook
rinpol	945.20		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	946.80		NIST Webbook
tb	435.70	K	KDB
tc	612.80	K	KDB
tf	219.00	K	KDB
vc	0.547	m3/kmol	KDB
zc	0.2404810		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.75	J/mol×K	571.35	Joback Method
cpg	376.87	J/mol×K	542.45	Joback Method
cpg	362.39	J/mol×K	513.56	Joback Method
cpg	347.31	J/mol×K	484.67	Joback Method
cpg	331.59	J/mol×K	455.77	Joback Method
cpg	315.23	J/mol×K	426.88	Joback Method
cpg	404.05	J/mol×K	600.24	Joback Method
dvisc	0.0495825	Pa×s	157.46	Joback Method
dvisc	0.0002081	Pa×s	426.88	Joback Method
dvisc	0.0003031	Pa×s	381.98	Joback Method
dvisc	0.0004880	Pa×s	337.07	Joback Method
dvisc	0.0009096	Pa×s	292.17	Joback Method
dvisc	0.0021254	Pa×s	247.27	Joback Method
dvisc	0.0072381	Pa×s	202.36	Joback Method
hvapt	37.45	kJ/mol	435.70	KDB
rfi	1.42060		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44018e+01
Coeff. B	-3.74439e+03
Coeff. C	-5.29330e+01
Temperature range (K), min.	318.23
Temperature range (K), max.	464.84

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.01903e+02
Coeff. B	-9.02814e+03

Coeff. C	-1.28511e+01
Coeff. D	8.06773e-06
Temperature range (K), min.	318.15
Temperature range (K), max.	612.80

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=141
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=141
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20278891&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

zc: Critical Compressibility