Heptane, 2,3,3-trimethyl-

Other names: 2,3,3-Trimethylheptane
Inchi: InChI=1S/C10H22/c1-6-7-8-10(4,5)9(2)3/h9H,6-8H2,1-5H3
InchiKey: QACXEXNKLFWKLK-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCCCC(C)(C)C(C)C
Mol. weight [g/mol]: 142.28
CAS: 52896-93-2

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	46.90	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	932.00		NIST Webbook
rinpol	931.70		NIST Webbook
rinpol	932.00		NIST Webbook
tb	433.20 ± 0.50	K	NIST Webbook
tc	600.93	K	Joback Method
tf	189.88	K	Joback Method
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	0.0206027	Pa×s	189.88	Joback Method
dvisc	0.0052013	Pa×s	228.99	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40851e+01
Coeff. B	-3.52747e+03
Coeff. C	-6.07420e+01
Temperature range (K), min.	316.40
Temperature range (K), max.	462.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.59724e+01
Coeff. B	-8.76860e+03
Coeff. C	-1.19258e+01
Coeff. D	6.84271e-06
Temperature range (K), min.	316.15
Temperature range (K), max.	617.50

Sources

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=130

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/files/research/kdb/mol/mol130.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52896932&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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume