Heptane, 3,3,4-trimethyl-

Other names: 3,3,4-Trimethylheptane
Inchi: InChI=1S/C10H22/c1-6-8-9(3)10(4,5)7-2/h9H,6-8H2,1-5H3
InchiKey: WRBHKVWLEIYLDZ-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCCC(C)C(C)(C)CC
Mol. weight [g/mol]: 142.28
CAS: 20278-87-9

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	36.17	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	937.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	936.30		NIST Webbook
rinpol	936.60		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook
tb	424.53	K	Joback Method
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*ln(T) + D*T^2
Coeff. A	9.36132e+01
Coeff. B	-8.66251e+03
Coeff. C	-1.15778e+01
Coeff. D	6.62643e-06
Temperature range (K), min.	317.15
Temperature range (K), max.	622.10

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=138

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20278879&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=138

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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