

Heptane, 2,5,5-trimethyl-

Other names:	2,5,5-Trimethylheptane
Inchi:	InChI=1S/C10H22/c1-6-10(4,5)8-7-9(2)3/h9H,6-8H2,1-5H3
InchiKey:	SOYLPZSOEXZMLE-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCC(C)(C)CCC(C)C
Mol. weight [g/mol]:	142.28
CAS:	1189-99-7

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	46.00	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	2161.32	kPa	Joback Method
rinpol	891.70		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	890.00		NIST Webbook
tb	425.95 ± 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
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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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40265e+01
Coeff. B	-3.40955e+03
Coeff. C	-6.35550e+01
Temperature range (K), min.	311.72
Temperature range (K), max.	454.78

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.96426e+01
Coeff. B	-8.85031e+03
Coeff. C	-1.24821e+01
Coeff. D	7.28843e-06
Temperature range (K), min.	312.15
Temperature range (K), max.	602.90

Sources

KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=137
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol137.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	https://webbook.nist.gov/cgi/cbook.cgi?ID=C1189997&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
nfpaf:	NFPA Fire Rating
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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