Pentane, 3,3-diethyl-2-methyl-

Other names:	2-Methyl-3,3-diethylpentane
	3,3-Diethyl-2-methylpentane
Inchi:	InChI=1S/C10H22/c1-6-10(7-2,8-3)9(4)5/h9H,6-8H2,1-5H3
InchiKey:	DSSAZLXYIQIXGW-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCC(CC)(CC)C(C)C
Mol. weight [g/mol]:	142.28
CAS:	52897-16-2

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	47.30	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	984.00		NIST Webbook
rinpol	984.00		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	394.47	J/mol×K	571.53	Joback Method
cpg	380.41	J/mol×K	542.13	Joback Method
cpg	365.66	J/mol×K	512.73	Joback Method
cpg	350.18	J/mol×K	483.33	Joback Method

cpg	333.94	J/mol×K	453.93	Joback Method
cpg	407.85	J/mol×K	600.93	Joback Method
dvisc	0.0002394	Pa×s	424.53	Joback Method
dvisc	0.0003452	Pa×s	385.42	Joback Method
dvisc	0.0005405	Pa×s	346.31	Joback Method
dvisc	0.0009486	Pa×s	307.20	Joback Method
dvisc	0.0019620	Pa×s	268.10	Joback Method
dvisc	0.0052013	Pa×s	228.99	Joback Method
dvisc	0.0206027	Pa×s	189.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41881e+01
Coeff. B	-3.72045e+03
Coeff. C	-5.40880e+01
Temperature range (K), min.	321.74
Temperature range (K), max.	473.22

Sources

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/mol166.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52897162&Units=SI

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

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

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