Pentane, 2,2,3,4,4-pentamethyl-

Other names: 2,2,3,4,4-Pentamethylpentane
Inchi: InChI=1S/C10H22/c1-8(9(2,3)4)10(5,6)7/h8H,1-7H3
InchiKey: OWFKEHICSVOVAC-UHFFFAOYSA-N
Formula: C10H22
SMILES: CC(C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 142.28
CAS: 16747-45-8

Physical Properties

Property code	Value	Unit	Source
af	0.3080		KDB
gf	36.56	kJ/mol	Joback Method
hcg	6786.03	kJ/mol	KDB
hcn	6301.941	kJ/mol	KDB
hf	-272.51	kJ/mol	Joback Method
hfus	3.30	kJ/mol	Joback Method
hvap	43.50	kJ/mol	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.715		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2400.00	kPa	KDB
rinpol	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	921.70		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
tb	432.44 ± 0.10	K	NIST Webbook
tb	432.50	K	KDB
tc	627.30	K	KDB
tf	234.00	K	KDB
tf	234.34 ± 0.10	K	NIST Webbook
vc	0.521	m3/kmol	KDB
zc	0.2397380		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.19	J/mol×K	577.94	Joback Method
cpg	387.32	J/mol×K	546.61	Joback Method
cpg	371.56	J/mol×K	515.28	Joback Method
cpg	354.85	J/mol×K	483.95	Joback Method
cpg	337.16	J/mol×K	452.63	Joback Method
cpg	318.44	J/mol×K	421.30	Joback Method
cpg	416.21	J/mol×K	609.26	Joback Method
dvisc	0.0381243	Pa×s	192.30	Joback Method
dvisc	0.0002554	Pa×s	421.30	Joback Method
dvisc	0.0003882	Pa×s	383.13	Joback Method
dvisc	0.0006474	Pa×s	344.97	Joback Method
dvisc	0.0012262	Pa×s	306.80	Joback Method
dvisc	0.0027843	Pa×s	268.63	Joback Method
dvisc	0.0082957	Pa×s	230.47	Joback Method
hvapt	35.31	kJ/mol	432.50	KDB
rfi	1.42868		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39890e+01
Coeff. B	-3.55716e+03
Coeff. C	-5.28460e+01
Temperature range (K), min.	312.47
Temperature range (K), max.	462.77

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.46751e+01
Coeff. B	-7.93986e+03
Coeff. C	-1.03629e+01

Coeff. D	6.42561e-06
Temperature range (K), min.	311.15
Temperature range (K), max.	627.30

Sources

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/mol171.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16747458&Units=SI
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=171

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