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

Other names: 2,2,3,3,4-Pentamethylpentane
2,2,3,3,4-Tetramethylpentane
Inchi: InChI=1S/C10H22/c1-8(2)10(6,7)9(3,4)5/h8H,1-7H3
InchiKey: WKQBIIUOSATALN-UHFFFAOYSA-N
Formula: C10H22
SMILES: CC(C)C(C)(C)C(C)(C)C
Mol. weight [g/mol]: 142.28
CAS: 16747-44-7

Physical Properties

Property code	Value	Unit	Source
gf	36.56	kJ/mol	Joback Method
hf	-272.51	kJ/mol	Joback Method
hfus	3.30	kJ/mol	Joback Method
hvap	45.20	kJ/mol	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.715		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	953.00		NIST Webbook
rinpol	949.40		NIST Webbook
rinpol	953.10		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	953.40		NIST Webbook
rinpol	953.00		NIST Webbook
tb	439.20 ± 0.10	K	NIST Webbook
tc	609.26	K	Joback Method
tf	236.66 ± 0.10	K	NIST Webbook
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.44	J/mol×K	421.30	Joback Method
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	416.21	J/mol×K	609.26	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
dvisc	0.0381243	Pa×s	192.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39464e+01
Coeff. B	-3.56589e+03
Coeff. C	-5.69360e+01
Temperature range (K), min.	318.00
Temperature range (K), max.	469.90

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol170.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16747447&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

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