Pentane, 3-ethyl-2,2,3-trimethyl-

Other names: 2,2,3-Trimethyl-3-ethylpentane
3-Ethyl-2,2,3-trimethylpentane
Inchi: InChI=1S/C10H22/c1-7-10(6,8-2)9(3,4)5/h7-8H2,1-6H3
InchiKey: AJDIFHIHSYVDGP-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCC(C)(CC)C(C)(C)C
Mol. weight [g/mol]: 142.28
CAS: 52897-17-3

Physical Properties

Property code	Value	Unit	Source
gf	39.00	kJ/mol	Joback Method
hf	-267.23	kJ/mol	Joback Method
hfus	6.83	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
pc	2183.60	kPa	Joback Method
rinpol	966.00		NIST Webbook
rinpol	967.30		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	965.70		NIST Webbook
rinpol	966.00		NIST Webbook
tb	421.74	K	Joback Method
tc	605.42	K	Joback Method
tf	230.90 ± 2.00	K	NIST Webbook
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.50	J/mol×K	421.74	Joback Method

cpg	336.71	J/mol×K	452.35	Joback Method
cpg	353.94	J/mol×K	482.97	Joback Method
cpg	370.23	J/mol×K	513.58	Joback Method
cpg	385.63	J/mol×K	544.19	Joback Method
cpg	400.18	J/mol×K	574.81	Joback Method
cpg	413.92	J/mol×K	605.42	Joback Method
dvisc	0.0186536	Pa×s	207.30	Joback Method
dvisc	0.0054554	Pa×s	243.04	Joback Method
dvisc	0.0021867	Pa×s	278.78	Joback Method
dvisc	0.0010789	Pa×s	314.52	Joback Method
dvisc	0.0006149	Pa×s	350.26	Joback Method
dvisc	0.0003889	Pa×s	386.00	Joback Method
dvisc	0.0002658	Pa×s	421.74	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40807e+01
Coeff. B	-3.70401e+03
Coeff. C	-5.12120e+01
Temperature range (K), min.	319.75
Temperature range (K), max.	473.60

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/mol167.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52897173&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