pentane, 3-ethyl-2,2,4-trimethyl-

Other names: 2,2,4-Trimethyl-3-ethylpentane
3-Ethyl-2,2,4-trimethylpentane
Inchi: InChI=1S/C10H22/c1-7-9(8(2)3)10(4,5)6/h8-9H,7H2,1-6H3
InchiKey: VLIZIVHXZXQRDE-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCC(C(C)C)C(C)(C)C
Mol. weight [g/mol]: 142.29
CAS: 52897-18-4

Physical Properties

Property code	Value	Unit	Source
af	0.3214		Cheméo Relay (1.0)
gf	31.28	kJ/mol	Joback Method
hf	-230.50	kJ/mol	Cheméo Relay (1.0)
hfus	7.20	kJ/mol	Joback Method
hvap	44.80	kJ/mol	NIST Webbook
log10ws	-5.10		Cheméo Relay (1.0)
logp	3.715		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	903.90		NIST Webbook
rinpol	901.20		NIST Webbook
tb	428.45 ± 0.40	K	NIST Webbook
tc	597.12	K	Cheméo Relay (1.0)
tf	170.45	K	Cheméo Relay (1.0)
vc	0.517	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.88	J/mol×K	424.09	Joback Method
cpg	334.37	J/mol×K	454.16	Joback Method
cpg	351.04	J/mol×K	484.23	Joback Method
cpg	366.91	J/mol×K	514.30	Joback Method
cpg	382.02	J/mol×K	544.37	Joback Method
cpg	396.39	J/mol×K	574.44	Joback Method
cpg	410.05	J/mol×K	604.51	Joback Method
dvisc	0.0446565	Pa×s	174.88	Joback Method
dvisc	0.0079881	Pa×s	216.41	Joback Method
dvisc	0.0024872	Pa×s	257.95	Joback Method
dvisc	0.0010703	Pa×s	299.49	Joback Method
dvisc	0.0005656	Pa×s	341.02	Joback Method
dvisc	0.0003433	Pa×s	382.55	Joback Method
dvisc	0.0002298	Pa×s	424.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40636e+01
Coeff. B	-3.52222e+03
Coeff. C	-5.55490e+01
Temperature range (K), min.	311.23
Temperature range (K), max.	457.99

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52897184&Units=SI

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

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

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

Legend

af:	Acentric Factor
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