Hexane, 3-ethyl-4,4-dimethyl

Other names: 3,3-Dimethyl-4-ethylhexane
4-Ethyl-3,3-dimethylhexane
Inchi: InChI=1S/C10H22/c1-6-9(7-2)10(4,5)8-3/h9H,6-8H2,1-5H3
InchiKey: ZRTXVJYJVBTXHE-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCC(CC)C(C)(C)CC
Mol. weight [g/mol]: 142.29
CAS: 52897-05-9

Physical Properties

Property code	Value	Unit	Source
af	0.3544		Cheméo Relay (1.0)
gf	33.72	kJ/mol	Joback Method
hf	-243.74	kJ/mol	Cheméo Relay (1.0)
hfus	10.72	kJ/mol	Joback Method
hvap	46.40	kJ/mol	NIST Webbook
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	938.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	937.80		NIST Webbook
rinpol	938.00		NIST Webbook
tb	435.44	K	Cheméo Relay (1.0)
tc	615.93	K	Cheméo Relay (1.0)
tf	184.23	K	Cheméo Relay (1.0)
vc	0.521	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.93	J/mol×K	424.53	Joback Method
cpg	333.94	J/mol×K	453.93	Joback Method

cpg	350.18	J/mol×K	483.33	Joback Method
cpg	365.66	J/mol×K	512.73	Joback Method
cpg	380.41	J/mol×K	542.13	Joback Method
cpg	394.47	J/mol×K	571.53	Joback Method
cpg	407.85	J/mol×K	600.93	Joback Method
dvisc	0.0206027	Pa×s	189.88	Joback Method
dvisc	0.0052013	Pa×s	228.99	Joback Method
dvisc	0.0019620	Pa×s	268.10	Joback Method
dvisc	0.0009486	Pa×s	307.20	Joback Method
dvisc	0.0005405	Pa×s	346.31	Joback Method
dvisc	0.0003452	Pa×s	385.42	Joback Method
dvisc	0.0002394	Pa×s	424.53	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41479e+01
Coeff. B	-3.61870e+03
Coeff. C	-5.63280e+01
Temperature range (K), min.	317.41
Temperature range (K), max.	465.85

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol152.mol

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52897059&Units=SI

Cheméo Relay (1.0):

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

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

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
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