

Heptane, 4-ethyl-3-methyl-

Other names:	3-Methyl-4-ethylheptane 4-Ethyl-3-methylheptane
Inchi:	InChI=1S/C10H22/c1-5-8-10(7-3)9(4)6-2/h9-10H,5-8H2,1-4H3
InchiKey:	BTGGSWBKRYMHQK-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCCC(CC)C(C)CC
Mol. weight [g/mol]:	142.28
CAS:	52896-89-6

Physical Properties

Property code	Value	Unit	Source
gf	28.44	kJ/mol	Joback Method
hf	-260.29	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	47.70	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	936.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	935.70		NIST Webbook
tb	427.32	K	Joback Method
tc	596.92	K	Joback Method
tf	172.46	K	Joback Method
vc	0.584	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.26	J/molxK	427.32	Joback Method

cpg	388.93	J/molxK	568.65	Joback Method
cpg	375.35	J/molxK	540.39	Joback Method
cpg	361.21	J/molxK	512.12	Joback Method
cpg	346.50	J/molxK	483.85	Joback Method
cpg	331.18	J/molxK	455.59	Joback Method
cpg	401.95	J/molxK	596.92	Joback Method
dvisc	0.0002171	Paxs	427.32	Joback Method
dvisc	0.0003059	Paxs	384.84	Joback Method
dvisc	0.0004693	Paxs	342.37	Joback Method
dvisc	0.0008129	Paxs	299.89	Joback Method
dvisc	0.0016877	Paxs	257.41	Joback Method
dvisc	0.0046771	Paxs	214.94	Joback Method
dvisc	0.0214146	Paxs	172.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43119e+01
Coeff. B	-3.66568e+03
Coeff. C	-5.72050e+01
Temperature range (K), min.	318.58
Temperature range (K), max.	464.48

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Joback Method:

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C52896896&Units=SI>

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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