Heptane, 5-ethyl-2-methyl-

Other names: 2-Methyl-5-ethylheptane
5-ETHYL-2-METHYLHEPTANE
Heptane, 3-ethyl-6-methyl
Inchi: InChI=1S/C10H22/c1-5-10(6-2)8-7-9(3)4/h9-10H,5-8H2,1-4H3
InchiKey: DGEMPTLPTFNEHJ-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCC(CC)CCC(C)C
Mol. weight [g/mol]: 142.28
CAS: 13475-78-0

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	48.10	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	924.80		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	925.00		NIST Webbook
tb	427.32	K	Joback Method
tc	596.92	K	Joback Method
tf	172.46	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.26	J/mol×K	427.32	Joback Method
cpg	388.93	J/mol×K	568.65	Joback Method
cpg	375.35	J/mol×K	540.39	Joback Method
cpg	361.21	J/mol×K	512.12	Joback Method
cpg	346.50	J/mol×K	483.85	Joback Method
cpg	331.18	J/mol×K	455.59	Joback Method
cpg	401.95	J/mol×K	596.92	Joback Method
dvisc	0.0002171	Pa×s	427.32	Joback Method
dvisc	0.0003059	Pa×s	384.84	Joback Method
dvisc	0.0004693	Pa×s	342.37	Joback Method
dvisc	0.0008129	Pa×s	299.89	Joback Method
dvisc	0.0016877	Pa×s	257.41	Joback Method
dvisc	0.0046771	Pa×s	214.94	Joback Method
dvisc	0.0214146	Pa×s	172.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42627e+01
Coeff. B	-3.58549e+03
Coeff. C	-6.10910e+01
Temperature range (K), min.	317.65
Temperature range (K), max.	461.65

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.05026e+02
Coeff. B	-9.24741e+03
Coeff. C	-1.32662e+01
Coeff. D	7.93227e-06
Temperature range (K), min.	317.15

Temperature range (K), max.	606.70

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13475780&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=120
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/mol120.mol

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