Octane, 4-ethyl-

Other names: 4-Ethyloctane
Inchi: InChI=1S/C10H22/c1-4-7-9-10(6-3)8-5-2/h10H,4-9H2,1-3H3
InchiKey: NRJUFUBKIFIKFI-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCCCC(CC)CCC
Mol. weight [g/mol]: 142.28
CAS: 15869-86-0

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
gf	30.88	kJ/mol	Joback Method
hcg	6778.33	kJ/mol	KDB
hcn	6294.201	kJ/mol	KDB
hf	-255.01	kJ/mol	Joback Method
hfus	18.13	kJ/mol	Joback Method
hvap	48.10	kJ/mol	NIST Webbook
log10ws	-3.77		Crippen Method
logp	4.003		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	2180.00	kPa	KDB
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	956.10		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	956.10		NIST Webbook

rinpol	958.00		NIST Webbook
rinpol	951.50		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	956.20		NIST Webbook
rinpol	956.10		NIST Webbook
rinpol	966.20		NIST Webbook
rinpol	950.90		NIST Webbook
rinpol	958.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	952.00		NIST Webbook
tb	436.80	K	KDB
tb	436.51 ± 0.20	K	NIST Webbook
tc	609.60	K	KDB
tf	185.00	K	KDB
vc	0.552	m3/kmol	KDB
zc	0.2374180		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.16	J/mol×K	566.07	Joback Method
cpg	399.91	J/mol×K	593.73	Joback Method
cpg	315.29	J/mol×K	427.76	Joback Method
cpg	330.79	J/mol×K	455.42	Joback Method
cpg	345.71	J/mol×K	483.08	Joback Method
cpg	360.07	J/mol×K	510.75	Joback Method
cpg	373.88	J/mol×K	538.41	Joback Method
dvisc	0.0002265	Pa×s	427.76	Joback Method
dvisc	0.0003093	Pa×s	387.71	Joback Method
dvisc	0.0108083	Pa×s	187.46	Joback Method
dvisc	0.0032190	Pa×s	227.51	Joback Method
dvisc	0.0013777	Pa×s	267.56	Joback Method
dvisc	0.0007355	Pa×s	307.61	Joback Method
dvisc	0.0004537	Pa×s	347.66	Joback Method
hvapt	38.28	kJ/mol	436.80	KDB
rfi	1.41310		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43819e+01
Coeff. B	-3.68234e+03
Coeff. C	-5.96500e+01
Temperature range (K), min.	320.91
Temperature range (K), max.	465.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.08465e+02
Coeff. B	-9.48733e+03
Coeff. C	-1.37699e+01
Coeff. D	8.31899e-06
Temperature range (K), min.	321.15
Temperature range (K), max.	609.60

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/research/kdb/hcprop/showprop.php?cmpid=103

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15869860&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=103

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
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility