3-ethylnonane

Other names: Nonane, 3-ethyl
Inchi: InChI=1S/C11H24/c1-4-7-8-9-10-11(5-2)6-3/h11H,4-10H2,1-3H3
InchiKey: FKJSIWPQZCKMIL-UHFFFAOYSA-N
Formula: C11H24
SMILES: CCCCCCC(CC)CC
Mol. weight [g/mol]: 156.31
CAS: 17302-11-3

Physical Properties

Property code	Value	Unit	Source
af	0.4814		Cheméo Relay (1.0)
gf	39.30	kJ/mol	Joback Method
hf	-269.28	kJ/mol	Cheméo Relay (1.0)
hfus	20.72	kJ/mol	Joback Method
hvap	51.25	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-5.96		Cheméo Relay (1.0)
logp	4.393		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
tb	458.95	K	Cheméo Relay (1.0)
tc	628.16	K	Cheméo Relay (1.0)
tf	192.72	K	Cheméo Relay (1.0)
vc	0.618	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.10	J/mol×K	450.64	Joback Method
cpg	376.48	J/mol×K	478.16	Joback Method
cpg	392.24	J/mol×K	505.68	Joback Method
cpg	407.41	J/mol×K	533.20	Joback Method
cpg	421.98	J/mol×K	560.73	Joback Method
cpg	435.99	J/mol×K	588.25	Joback Method

cpg	449.44	J/mol×K	615.77	Joback Method
dvisc	0.0105797	Pa×s	198.73	Joback Method
dvisc	0.0031400	Pa×s	240.72	Joback Method
dvisc	0.0013369	Pa×s	282.70	Joback Method
dvisc	0.0007098	Pa×s	324.69	Joback Method
dvisc	0.0004357	Pa×s	366.67	Joback Method
dvisc	0.0002956	Pa×s	408.65	Joback Method
dvisc	0.0002156	Pa×s	450.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41465e+01
Coeff. B	-3.57973e+03
Coeff. C	-8.54500e+01
Temperature range (K), min.	343.75
Temperature range (K), max.	490.63

Sources

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

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=C17302113&Units=SI

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume