1-Ethyl-2-methylcyclohexane

Inchi: InChI=1S/C9H18/c1-3-9-7-5-4-6-8(9)2/h8-9H,3-7H2,1-2H3
InchiKey: XARGIVYWQPXRTC-UHFFFAOYSA-N
Formula: C9H18
SMILES: CCC1CCCCC1C
Mol. weight [g/mol]: 126.24
CAS: 3728-54-9

Physical Properties

Property code	Value	Unit	Source
af	0.2640		Cheméo Relay (1.0)
gf	41.64	kJ/mol	Joback Method
hf	-181.78	kJ/mol	Cheméo Relay (1.0)
hfus	11.97	kJ/mol	Joback Method
hvap	42.34	kJ/mol	Cheméo Relay (1.0)
ie	9.38	eV	Cheméo Relay (1.0)
log10ws	-4.89		Cheméo Relay (1.0)
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	919.00		NIST Webbook
rinpol	919.00		NIST Webbook
tb	426.80 ± 3.00	K	NIST Webbook
tb	424.20	K	NIST Webbook
tc	621.78	K	Cheméo Relay (1.0)
tf	166.95	K	Cheméo Relay (1.0)
vc	0.444	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.07	J/mol×K	420.20	Joback Method
cpg	273.91	J/mol×K	453.28	Joback Method
cpg	291.90	J/mol×K	486.37	Joback Method
cpg	309.07	J/mol×K	519.45	Joback Method

cpg	325.42	J/mol×K	552.53	Joback Method
cpg	340.98	J/mol×K	585.62	Joback Method
cpg	355.76	J/mol×K	618.70	Joback Method
dvisc	0.0046654	Pa×s	194.33	Joback Method
dvisc	0.0019666	Pa×s	231.97	Joback Method
dvisc	0.0010552	Pa×s	269.62	Joback Method
dvisc	0.0006594	Pa×s	307.26	Joback Method
dvisc	0.0004567	Pa×s	344.91	Joback Method
dvisc	0.0003400	Pa×s	382.56	Joback Method
dvisc	0.0002668	Pa×s	420.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44629e+01
Coeff. B	-3.59289e+03
Coeff. C	-5.94390e+01
Temperature range (K), min.	312.90
Temperature range (K), max.	452.04

Sources

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=C3728549&Units=SI

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

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

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