trans-4-Ethyl cyclohexanol

Other names:	4-Ethylcyclohexanol,c&t
	4-ethylcyclohexanol
	Cyclohexanol, 4-ethyl-
Inchi:	InChI=1S/C8H16O/c1-2-7-3-5-8(9)6-4-7/h7-9H,2-6H2,1H3
InchiKey:	RVTKUJWGFBADIN-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CCC1CCC(O)CC1
Mol. weight [g/mol]:	128.21
CAS:	4534-74-1

Physical Properties

Property code	Value	Unit	Source
af	0.4869		Cheméo Relay (1.0)
gf	-103.60	kJ/mol	Joback Method
hf	-319.91	kJ/mol	Cheméo Relay (1.0)
hfus	13.47	kJ/mol	Joback Method
hvap	71.85	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
log10ws	-1.67		Cheméo Relay (1.0)
logp	1.948		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1003.00		NIST Webbook
tb	465.00 ± 3.00	K	NIST Webbook
tc	663.03	K	Cheméo Relay (1.0)
tf	264.85	K	Cheméo Relay (1.0)
vc	0.418	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.40	J/mol×K	489.50	Joback Method
cpg	290.58	J/mol×K	521.21	Joback Method
cpg	305.05	J/mol×K	552.93	Joback Method

cpg	318.84	J/mol×K	584.64	Joback Method
cpg	331.95	J/mol×K	616.35	Joback Method
cpg	344.40	J/mol×K	648.07	Joback Method
cpg	356.21	J/mol×K	679.78	Joback Method
dvisc	0.0447466	Pa×s	243.88	Joback Method
dvisc	0.0093317	Pa×s	284.82	Joback Method
dvisc	0.0028858	Pa×s	325.75	Joback Method
dvisc	0.0011598	Pa×s	366.69	Joback Method
dvisc	0.0005598	Pa×s	407.63	Joback Method
dvisc	0.0003086	Pa×s	448.56	Joback Method
dvisc	0.0001879	Pa×s	489.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38077e+01
Coeff. B	-3.66385e+03
Coeff. C	-6.21190e+01
Temperature range (K), min.	333.11
Temperature range (K), max.	493.35

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=C4534741&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume