1-ethyl-2-methylcyclohexanol

Inchi: InChI=1S/C9H18O/c1-3-9(10)7-5-4-6-8(9)2/h8,10H,3-7H2,1-2H3
InchiKey: YIXMIPVWEWDXSJ-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCC1(O)CCCCC1C
Mol. weight [g/mol]: 142.24
CAS: 102370-18-3

Physical Properties

Property code	Value	Unit	Source
hfus	9.76	kJ/mol	Joback Method
ie	9.28	eV	Cheméo Relay (1.0)
logp	2.338		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
tb	456.58	K	Cheméo Relay (1.0)
tf	265.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.47	J/mol×K	512.62	Joback Method
cpg	337.38	J/mol×K	545.22	Joback Method
cpg	352.40	J/mol×K	577.81	Joback Method
cpg	366.59	J/mol×K	610.41	Joback Method
cpg	380.04	J/mol×K	643.00	Joback Method
cpg	392.82	J/mol×K	675.60	Joback Method
cpg	405.03	J/mol×K	708.19	Joback Method

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37225e+01
Coeff. B	-3.78111e+03
Coeff. C	-6.76820e+01
Temperature range (K), min.	310.05
Temperature range (K), max.	517.22

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102370183&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point