

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:	32296-45-0

Physical Properties

Property code	Value	Unit	Source
gf	-100.67	kJ/mol	Joback Method
hf	-332.10	kJ/mol	Joback Method
hfus	9.76	kJ/mol	Joback Method
hvap	51.28	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.338		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	512.62	K	Joback Method
tc	708.19	K	Joback Method
tf	279.05	K	Joback Method
vc	0.488	m3/kmol	Joback Method

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	$\ln(P_{vp}) = A + B/(T + C)$
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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32296450&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
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

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