

Cyclohexanol, 1-propyl-

Other names:	1-Propylcyclohexanol 1-n-Propylcyclohexanol
Inchi:	InChI=1S/C9H18O/c1-2-6-9(10)7-4-3-5-8-9/h10H,2-8H2,1H3
InchiKey:	PYLPYOPJKOJRNP-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CCCC1(O)CCCCC1
Mol. weight [g/mol]:	142.24
CAS:	5445-24-9

Physical Properties

Property code	Value	Unit	Source
gf	-92.96	kJ/mol	Joback Method
hf	-311.76	kJ/mol	Joback Method
hfus	8.69	kJ/mol	Joback Method
hvap	51.59	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.482		Crippen Method
mvol	132.680	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	453.00 ± 4.00	K	NIST Webbook
tc	713.09	K	Joback Method
tf	283.29	K	Joback Method
vc	0.489	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.65	J/mol×K	517.29	Joback Method
cpg	336.17	J/mol×K	549.92	Joback Method
cpg	350.77	J/mol×K	582.56	Joback Method
cpg	364.56	J/mol×K	615.19	Joback Method
cpg	377.60	J/mol×K	647.82	Joback Method
cpg	389.99	J/mol×K	680.46	Joback Method
cpg	401.82	J/mol×K	713.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38284e+01
Coeff. B	-3.82131e+03
Coeff. C	-6.80910e+01
Temperature range (K), min.	350.30
Temperature range (K), max.	516.76

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5445249&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/ci9903071
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

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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