

Cyclopentane, 1,1-diethyl-

Other names:	1,1-diethylcyclopentane
Inchi:	InChI=1S/C9H18/c1-3-9(4-2)7-5-6-8-9/h3-8H2,1-2H3
InchiKey:	DPGQSDLGKGLNHC-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CCC1(CC)CCCC1
Mol. weight [g/mol]:	126.24
CAS:	2721-38-2

Physical Properties

Property code	Value	Unit	Source
gf	55.96	kJ/mol	Joback Method
hf	-153.37	kJ/mol	Joback Method
hfus	6.70	kJ/mol	Joback Method
hvap	34.73	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.367		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
tb	420.84	K	Joback Method
tc	620.53	K	Joback Method
tf	225.99	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.85	J/mol×K	420.84	Joback Method
cpg	275.03	J/mol×K	454.12	Joback Method
cpg	292.03	J/mol×K	487.40	Joback Method
cpg	307.94	J/mol×K	520.68	Joback Method
cpg	322.85	J/mol×K	553.96	Joback Method
cpg	336.87	J/mol×K	587.24	Joback Method
cpg	350.08	J/mol×K	620.53	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40837e+01
Coeff. B	-3.40590e+03
Coeff. C	-6.27450e+01
Temperature range (K), min.	309.62
Temperature range (K), max.	451.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2721382&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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol518.mol
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
log_{10ws}:	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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