

1,4-Pentadien-3-ol

Other names:	penta-1,4-dien-3-ol
Inchi:	InChI=1S/C5H8O/c1-3-5(6)4-2/h3-6H,1-2H2
InchiKey:	ICMWSAALRSINTC-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C=CC(O)C=C
Mol. weight [g/mol]:	84.12
CAS:	922-65-6

Physical Properties

Property code	Value	Unit	Source
gf	27.64	kJ/mol	Joback Method
hf	-53.18	kJ/mol	Joback Method
hfus	6.71	kJ/mol	Joback Method
hvap	41.67	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	0.719		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	388.70	K	NIST Webbook
tc	570.88	K	Joback Method
tf	188.41	K	Joback Method
vc	0.290	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.66	J/mol×K	398.90	Joback Method
cpg	147.98	J/mol×K	427.56	Joback Method
cpg	154.95	J/mol×K	456.23	Joback Method
cpg	161.60	J/mol×K	484.89	Joback Method
cpg	167.92	J/mol×K	513.55	Joback Method
cpg	173.94	J/mol×K	542.22	Joback Method
cpg	179.68	J/mol×K	570.88	Joback Method
dvisc	0.2418615	Paxs	188.41	Joback Method

dvisc	0.0325216	Paxs	223.49	Joback Method
dvisc	0.0075375	Paxs	258.57	Joback Method
dvisc	0.0024774	Paxs	293.65	Joback Method
dvisc	0.0010325	Paxs	328.74	Joback Method
dvisc	0.0005094	Paxs	363.82	Joback Method
dvisc	0.0002846	Paxs	398.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	338.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.59659e+01
Coeff. B	-3.85254e+03
Coeff. C	-4.91950e+01
Temperature range (K), min.	294.92
Temperature range (K), max.	410.79

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C922656&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

Legend

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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