4-Penten-1-ol

Other names:	4-Pentene-1-ol
	4-Pentenol
	4-Pentenyl alcohol
	CH2=CHCH2CH2CH2OH
	Pent-4-en-1-ol
Inchi:	InChI=1S/C5H10O/c1-2-3-4-5-6/h2,6H,1,3-5H2
InchiKey:	LQAVWYMTUMSFBE-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	C=CCCCO
Mol. weight [g/mol]:	86.13
CAS:	821-09-0

Physical Properties

Property code	Value	Unit	Source
gf	-57.76	kJ/mol	Joback Method
hf	-173.33	kJ/mol	Joback Method
hfus	11.51	kJ/mol	Joback Method
hvap	42.73	kJ/mol	Joback Method
ie	9.42 ± 0.05	eV	NIST Webbook
log10ws	-0.15		Aqueous Solubility Prediction Method
log10ws	-0.15		Estimated Solubility Method
logp	0.945		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
rinpol	757.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	717.00		NIST Webbook
ripol	1297.00		NIST Webbook

ripol	1289.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1295.00		NIST Webbook
ripol	1294.00		NIST Webbook
tb	408.70	K	NIST Webbook
tb	414.20	K	NIST Webbook
tb	408.00 ± 3.00	K	NIST Webbook
tb	413.00 ± 5.00	K	NIST Webbook
tc	567.49	K	Joback Method
tf	205.17	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.12	J/mol×K	402.66	Joback Method
cpg	190.73	J/mol×K	540.02	Joback Method
cpg	184.19	J/mol×K	512.54	Joback Method
cpg	177.36	J/mol×K	485.07	Joback Method
cpg	170.25	J/mol×K	457.60	Joback Method
cpg	162.84	J/mol×K	430.13	Joback Method
cpg	197.00	J/mol×K	567.49	Joback Method
dvisc	0.0002939	Pa×s	402.66	Joback Method
dvisc	0.0005036	Pa×s	369.75	Joback Method
dvisc	0.0009587	Pa×s	336.83	Joback Method
dvisc	0.0020980	Pa×s	303.91	Joback Method
dvisc	0.0055532	Pa×s	271.00	Joback Method
dvisc	0.0192385	Pa×s	238.09	Joback Method
dvisc	0.0992986	Pa×s	205.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59002e+01
Coeff. B	-3.99316e+03
Coeff. C	-5.47550e+01
Temperature range (K), min.	287.34
Temperature range (K), max.	431.87

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C821090&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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume