1,4-PENTANEDIOL

Other names: pentane-1,4-diol
Inchi: InChI=1S/C5H12O2/c1-5(7)3-2-4-6/h5-7H,2-4H2,1H3
InchiKey: GLOBUAZSRIOKLN-UHFFFAOYSA-N
Formula: C5H12O2
SMILES: CC(O)CCCO
Mol. weight [g/mol]: 104.15
CAS: 626-95-9

Physical Properties

Property code	Value	Unit	Source
af	0.7009		Cheméo Relay (1.0)
gf	-284.86	kJ/mol	Joback Method
hf	-471.23	kJ/mol	Cheméo Relay (1.0)
hfus	13.36	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Cheméo Relay (1.0)
ie	9.92	eV	Cheméo Relay (1.0)
log10ws	0.49		Cheméo Relay (1.0)
logp	0.140		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	479.22	K	Cheméo Relay (1.0)
tc	671.44	K	Cheméo Relay (1.0)
tf	259.16	K	Cheméo Relay (1.0)
vc	0.346	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.31	J/mol×K	497.72	Joback Method
cpg	220.99	J/mol×K	524.53	Joback Method
cpg	228.37	J/mol×K	551.34	Joback Method
cpg	235.47	J/mol×K	578.15	Joback Method
cpg	242.28	J/mol×K	604.96	Joback Method
cpg	248.82	J/mol×K	631.77	Joback Method

cpg	255.10	J/mol×K	658.58	Joback Method
dvisc	0.3861453	Pa×s	252.75	Joback Method
dvisc	0.0370842	Pa×s	293.58	Joback Method
dvisc	0.0063110	Pa×s	334.41	Joback Method
dvisc	0.0015790	Pa×s	375.24	Joback Method
dvisc	0.0005185	Pa×s	416.06	Joback Method
dvisc	0.0002078	Pa×s	456.89	Joback Method
dvisc	0.0000967	Pa×s	497.72	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56591e+01
Coeff. B	-4.51734e+03
Coeff. C	-7.32420e+01
Temperature range (K), min.	367.12
Temperature range (K), max.	509.80

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626959&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor

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