1,3-Pentanediol

Other names: pentane 1,3 diol
Inchi: InChI=1S/C5H12O2/c1-2-5(7)3-4-6/h5-7H,2-4H2,1H3
InchiKey: RUOPINZRYMFPBF-UHFFFAOYSA-N
Formula: C5H12O2
SMILES: CCC(O)CCO
Mol. weight [g/mol]: 104.15
CAS: 3174-67-2

Physical Properties

Property code	Value	Unit	Source
gf	-284.86	kJ/mol	Joback Method
hf	-456.27	kJ/mol	Joback Method
hfus	13.36	kJ/mol	Joback Method
hvap	59.69	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.140		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
tb	497.72	K	Joback Method
tc	658.58	K	Joback Method
tf	252.75	K	Joback Method
vc	0.347	m3/kmol	Joback Method

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	1.77652e+01
Coeff. B	-5.30964e+03
Coeff. C	-7.85240e+01
Temperature range (K), min.	382.32
Temperature range (K), max.	504.87

Sources

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
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3174672&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume