1,2-Heptanediol

Inchi: InChI=1S/C7H16O2/c1-2-3-4-5-7(9)6-8/h7-9H,2-6H2,1H3
InchiKey: GCXZDAKFJKCPGK-UHFFFAOYSA-N
Formula: C7H16O2
SMILES: CCCCCC(O)CO
Mol. weight [g/mol]: 132.20
CAS: 3710-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-268.02	kJ/mol	Joback Method
hf	-497.55	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.920		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1065.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1470.00		NIST Webbook
tb	543.48	K	Joback Method
tc	703.08	K	Joback Method
tf	275.29	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.37	J/mol×K	543.48	Joback Method
cpg	308.91	J/mol×K	570.08	Joback Method
cpg	318.08	J/mol×K	596.68	Joback Method
cpg	326.88	J/mol×K	623.28	Joback Method

cpg	335.33	J/mol×K	649.88	Joback Method
cpg	343.43	J/mol×K	676.48	Joback Method
cpg	351.20	J/mol×K	703.08	Joback Method
dvisc	0.1642467	Pa×s	275.29	Joback Method
dvisc	0.0172033	Pa×s	319.99	Joback Method
dvisc	0.0031328	Pa×s	364.69	Joback Method
dvisc	0.0008275	Pa×s	409.38	Joback Method
dvisc	0.0002841	Pa×s	454.08	Joback Method
dvisc	0.0001181	Pa×s	498.78	Joback Method
dvisc	0.0000567	Pa×s	543.48	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68850e+01
Coeff. B	-5.18952e+03
Coeff. C	-8.32500e+01
Temperature range (K), min.	395.92
Temperature range (K), max.	531.65

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3710314&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
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

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