2,4-Heptanediol

Inchi: InChI=1S/C7H16O2/c1-3-4-7(9)5-6(2)8/h6-9H,3-5H2,1-2H3
InchiKey: XVEOUOTUJBYHNL-UHFFFAOYSA-N
Formula: C7H16O2
SMILES: CCCC(O)CC(C)O
Mol. weight [g/mol]: 132.20
CAS: 20748-86-1

Physical Properties

Property code	Value	Unit	Source
gf	-270.46	kJ/mol	Joback Method
hf	-502.83	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	63.76	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.918		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	1051.00		NIST Webbook
tb	543.04	K	Joback Method
tc	705.35	K	Joback Method
tf	260.29	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.72	J/mol×K	543.04	Joback Method
cpg	309.47	J/mol×K	570.09	Joback Method
cpg	318.84	J/mol×K	597.14	Joback Method
cpg	327.82	J/mol×K	624.19	Joback Method
cpg	336.43	J/mol×K	651.24	Joback Method
cpg	344.68	J/mol×K	678.30	Joback Method
cpg	352.58	J/mol×K	705.35	Joback Method
dvisc	0.4213623	Pa×s	260.29	Joback Method

dvisc	0.0300384	Pa×s	307.42	Joback Method
dvisc	0.0043212	Pa×s	354.54	Joback Method
dvisc	0.0009798	Pa×s	401.66	Joback Method
dvisc	0.0003034	Pa×s	448.79	Joback Method
dvisc	0.0001174	Pa×s	495.91	Joback Method
dvisc	0.0000536	Pa×s	543.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.70	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65701e+01
Coeff. B	-5.06608e+03
Coeff. C	-8.24320e+01
Temperature range (K), min.	393.57
Temperature range (K), max.	532.40

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20748861&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

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