2-Methyl-2,3-pentanediol

Inchi: InChI=1S/C6H14O2/c1-4-5(7)6(2,3)8/h5,7-8H,4H2,1-3H3
InchiKey: GSQFUEPQVUSAPE-UHFFFAOYSA-N
Formula: C6H14O2
SMILES: CCC(O)C(C)(C)O
Mol. weight [g/mol]: 118.17
CAS: 7795-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-273.60	kJ/mol	Joback Method
hf	-485.66	kJ/mol	Joback Method
hfus	8.53	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	0.528		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	467.65 ± 2.00	K	NIST Webbook
tc	685.89	K	Joback Method
tf	266.44	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.90	J/mol×K	517.37	Joback Method
cpg	268.16	J/mol×K	545.46	Joback Method
cpg	276.95	J/mol×K	573.54	Joback Method
cpg	285.31	J/mol×K	601.63	Joback Method
cpg	293.24	J/mol×K	629.72	Joback Method
cpg	300.78	J/mol×K	657.80	Joback Method
cpg	307.94	J/mol×K	685.89	Joback Method
dvisc	0.3110979	Pa×s	266.44	Joback Method
dvisc	0.0300065	Pa×s	308.26	Joback Method

dvisc	0.0050606	Pa×s	350.08	Joback Method
dvisc	0.0012479	Pa×s	391.90	Joback Method
dvisc	0.0004031	Pa×s	433.73	Joback Method
dvisc	0.0001588	Pa×s	475.55	Joback Method
dvisc	0.0000728	Pa×s	517.37	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76162e+01
Coeff. B	-5.36937e+03
Coeff. C	-8.17510e+01
Temperature range (K), min.	391.61
Temperature range (K), max.	518.12

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=C7795804&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume