3-methyl-1,3-butanediol

Inchi: InChI=1S/C5H12O2/c1-5(2,7)3-4-6/h6-7H,3-4H2,1-2H3
InchiKey: XPFCZYUVICHKDS-UHFFFAOYSA-N
Formula: C5H12O2
SMILES: CC(C)(O)CCO
Mol. weight [g/mol]: 104.15
CAS: 2568-33-4

Physical Properties

Property code	Value	Unit	Source
hf	-490.35	kJ/mol	Cheméo Relay (1.0)
hfus	9.47	kJ/mol	Joback Method
hvap	71.87	kJ/mol	Cheméo Relay (1.0)
ie	9.91	eV	Cheméo Relay (1.0)
log10ws	0.72		Cheméo Relay (1.0)
logp	0.140		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4474.22	kPa	Joback Method
tb	476.65	K	Cheméo Relay (1.0)
tc	656.44	K	Cheméo Relay (1.0)
tf	286.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.54	J/mol×K	494.93	Joback Method
cpg	259.45	J/mol×K	661.34	Joback Method
cpg	253.18	J/mol×K	633.61	Joback Method
cpg	246.59	J/mol×K	605.87	Joback Method
cpg	239.64	J/mol×K	578.14	Joback Method
cpg	232.33	J/mol×K	550.40	Joback Method
cpg	224.63	J/mol×K	522.67	Joback Method
dvisc	0.0014473	Pa×s	382.55	Joback Method
dvisc	0.0001025	Pa×s	494.93	Joback Method
dvisc	0.0002144	Pa×s	457.47	Joback Method

dvisc	0.0005115	Pa×s	420.01	Joback Method
dvisc	0.1849815	Pa×s	270.17	Joback Method
dvisc	0.0051321	Pa×s	345.09	Joback Method
dvisc	0.0247700	Pa×s	307.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53763e+01
Coeff. B	-4.41060e+03
Coeff. C	-7.24080e+01
Temperature range (K), min.	364.72
Temperature range (K), max.	510.63

Sources

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

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

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

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

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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