2,3,3-Trimethyl-2-pentanol

Inchi: InChI=1S/C8H18O/c1-6-7(2,3)8(4,5)9/h9H,6H2,1-5H3
InchiKey: FBWWGYIEJGQWJP-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCC(C)(C)C(C)(C)O
Mol. weight [g/mol]: 130.23
CAS: 23171-85-9

Physical Properties

Property code	Value	Unit	Source
gf	-114.66	kJ/mol	Joback Method
hf	-378.18	kJ/mol	Joback Method
hfus	5.74	kJ/mol	Joback Method
hvap	47.49	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
tb	468.16	K	Joback Method
tc	647.15	K	Joback Method
tf	245.58	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.54	J/mol×K	468.16	Joback Method
cpg	309.17	J/mol×K	497.99	Joback Method
cpg	322.04	J/mol×K	527.82	Joback Method
cpg	334.18	J/mol×K	557.66	Joback Method
cpg	345.63	J/mol×K	587.49	Joback Method
cpg	356.43	J/mol×K	617.32	Joback Method
cpg	366.61	J/mol×K	647.15	Joback Method
dvisc	0.1025795	Pa×s	245.58	Joback Method
dvisc	0.0179252	Pa×s	282.68	Joback Method

dvisc	0.0046951	Pa×s	319.77	Joback Method
dvisc	0.0016247	Pa×s	356.87	Joback Method
dvisc	0.0006866	Pa×s	393.97	Joback Method
dvisc	0.0003365	Pa×s	431.06	Joback Method
dvisc	0.0001847	Pa×s	468.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52255e+01
Coeff. B	-4.46168e+03
Coeff. C	-2.34840e+01
Temperature range (K), min.	322.17
Temperature range (K), max.	473.52

Sources

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=C23171859&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

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