2-Hexanol, 2,5-dimethyl-, (S)-

Other names:	2,5-Dimethyl-2-hexanol
	2,5-dimethylhexan-2-ol
	2-Hexanol, 2,5-dimethyl-
	2-Hexanol, 2,5-dimethyl-, (S)-(+)-
Inchi:	InChI=1S/C8H18O/c1-7(2)5-6-8(3,4)9/h7,9H,5-6H2,1-4H3
InchiKey:	JPUIYNHIEXIFMV-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CC(C)CCC(C)(C)O
Mol. weight [g/mol]:	130.23
CAS:	3730-60-7

Physical Properties

Property code	Value	Unit	Source
gf	-119.94	kJ/mol	Joback Method
hf	-374.71	kJ/mol	Joback Method
hfus	9.63	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	857.10		NIST Webbook
tb	428.15 ± 3.00	K	NIST Webbook
tb	426.15 ± 3.00	K	NIST Webbook
tb	426.65 ± 3.00	K	NIST Webbook
tb	421.15 ± 5.00	K	NIST Webbook
tb	427.15 ± 3.00	K	NIST Webbook
tc	643.32	K	Joback Method
tf	228.16	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	292.99	J/mol×K	470.95	Joback Method
cpg	305.85	J/mol×K	499.68	Joback Method
cpg	318.10	J/mol×K	528.41	Joback Method
cpg	329.77	J/mol×K	557.13	Joback Method
cpg	340.87	J/mol×K	585.86	Joback Method
cpg	351.43	J/mol×K	614.59	Joback Method
cpg	361.48	J/mol×K	643.32	Joback Method
dvisc	0.1736472	Pa×s	228.16	Joback Method
dvisc	0.0230030	Pa×s	268.62	Joback Method
dvisc	0.0051732	Pa×s	309.09	Joback Method
dvisc	0.0016435	Pa×s	349.55	Joback Method
dvisc	0.0006624	Pa×s	390.02	Joback Method
dvisc	0.0003167	Pa×s	430.49	Joback Method
dvisc	0.0001719	Pa×s	470.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46575e+01
Coeff. B	-3.19178e+03
Coeff. C	-1.08718e+02
Temperature range (K), min.	330.83
Temperature range (K), max.	450.23

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=C3730607&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume