5-Undecanol, 2-methyl-

Other names: 2-Methyl-5-undecanol
Inchi: InChI=1S/C12H26O/c1-4-5-6-7-8-12(13)10-9-11(2)3/h11-13H,4-10H2,1-3H3
InchiKey: IHRNKXOJQXUPBE-UHFFFAOYSA-N
Formula: C12H26O
SMILES: CCCCCCC(O)CCC(C)C
Mol. weight [g/mol]: 186.33
CAS: 33978-71-1

Physical Properties

Property code	Value	Unit	Source
gf	-91.54	kJ/mol	Joback Method
hf	-453.80	kJ/mol	Joback Method
hfus	23.88	kJ/mol	Joback Method
hvap	58.21	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.754		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
tb	565.26	K	Joback Method
tc	728.05	K	Joback Method
tf	255.82	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.00	J/mol×K	565.26	Joback Method
cpg	549.01	J/mol×K	700.92	Joback Method
cpg	536.16	J/mol×K	673.79	Joback Method
cpg	522.76	J/mol×K	646.65	Joback Method
cpg	508.77	J/mol×K	619.52	Joback Method
cpg	494.19	J/mol×K	592.39	Joback Method
cpg	561.31	J/mol×K	728.05	Joback Method
dvisc	0.0000761	Pa×s	565.26	Joback Method

dvisc	0.0001352	Pa×s	513.69	Joback Method
dvisc	0.0002731	Pa×s	462.11	Joback Method
dvisc	0.0006581	Pa×s	410.54	Joback Method
dvisc	0.0020420	Pa×s	358.97	Joback Method
dvisc	0.0092648	Pa×s	307.39	Joback Method
dvisc	0.0773422	Pa×s	255.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53070e+01
Coeff. B	-4.70696e+03
Coeff. C	-8.36340e+01
Temperature range (K), min.	397.03
Temperature range (K), max.	554.54

Sources

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=C33978711&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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