3-Dodecanol

Other names: (dl) 3-dodecanol
Inchi: InChI=1S/C12H26O/c1-3-5-6-7-8-9-10-11-12(13)4-2/h12-13H,3-11H2,1-2H3
InchiKey: OKDGZLITBCRLLJ-UHFFFAOYSA-N
Formula: C12H26O
SMILES: CCCCCCCCCC(O)CC
Mol. weight [g/mol]: 186.33
CAS: 10203-30-2

Physical Properties

Property code	Value	Unit	Source
gf	-89.10	kJ/mol	Joback Method
hf	-448.52	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.898		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1407.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1779.00		NIST Webbook
ripol	1769.00		NIST Webbook
tb	565.70	K	Joback Method
tc	725.92	K	Joback Method
tf	270.82	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.62	J/mol×K	725.92	Joback Method
cpg	478.70	J/mol×K	565.70	Joback Method
cpg	493.60	J/mol×K	592.40	Joback Method
cpg	507.92	J/mol×K	619.11	Joback Method

cpg	521.66	J/mol×K	645.81	Joback Method
cpg	534.85	J/mol×K	672.51	Joback Method
cpg	547.50	J/mol×K	699.22	Joback Method
dvisc	0.0000810	Pa×s	565.70	Joback Method
dvisc	0.0381702	Pa×s	270.82	Joback Method
dvisc	0.0062239	Pa×s	319.97	Joback Method
dvisc	0.0016449	Pa×s	369.11	Joback Method
dvisc	0.0005944	Pa×s	418.26	Joback Method
dvisc	0.0002660	Pa×s	467.41	Joback Method
dvisc	0.0001387	Pa×s	516.55	Joback Method
hvapt	78.30	kJ/mol	318.00	NIST Webbook

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10203302&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

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

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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume