2-Dodecanol

Other names: Dodecan-2-ol
Dodecanol-2
Inchi: InChI=1S/C12H26O/c1-3-4-5-6-7-8-9-10-11-12(2)13/h12-13H,3-11H2,1-2H3
InchiKey: XSWSEQPWKOWORN-UHFFFAOYSA-N
Formula: C12H26O
SMILES: CCCCCCCCCCC(C)O
Mol. weight [g/mol]: 186.33
CAS: 10203-28-8

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	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1806.00		NIST Webbook
tb	523.15 ± 3.00	K	NIST Webbook
tb	518.15 ± 3.00	K	NIST Webbook
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	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
cpg	559.62	J/mol×K	725.92	Joback Method
dvisc	0.0062239	Pa×s	319.97	Joback Method
dvisc	0.0381702	Pa×s	270.82	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
dvisc	0.0000810	Pa×s	565.70	Joback Method
hvapt	87.00	kJ/mol	343.00	NIST Webbook
hvapt	85.00	kJ/mol	318.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65664e+01
Coeff. B	-5.20887e+03
Coeff. C	-8.71420e+01
Temperature range (K), min.	407.12
Temperature range (K), max.	549.95

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=C10203288&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
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