1,11-UNDECANEDIOL

Other names: Undecane-1,11-diol
Inchi: InChI=1S/C11H24O2/c12-10-8-6-4-2-1-3-5-7-9-11-13/h12-13H,1-11H2
InchiKey: XSMIOONHPKRREI-UHFFFAOYSA-N
Formula: C11H24O2
SMILES: OCCCCCCCCCCCO
Mol. weight [g/mol]: 188.31
CAS: 765-04-8

Physical Properties

Property code	Value	Unit	Source
af	0.9645		Cheméo Relay (1.0)
gf	-231.90	kJ/mol	Joback Method
hf	-556.29	kJ/mol	Cheméo Relay (1.0)
hfus	32.42	kJ/mol	Joback Method
hvap	118.91	kJ/mol	Cheméo Relay (1.0)
ie	9.84	eV	Cheméo Relay (1.0)
log10ws	-3.46		Cheméo Relay (1.0)
logp	2.482		Crippen Method
mcvol	177.590	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
tb	574.16	K	Cheméo Relay (1.0)
tc	777.27	K	Cheméo Relay (1.0)
tf	334.10	K	Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect
tf	335.40 ± 1.50	K	NIST Webbook
vc	0.691	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	492.31	J/mol×K	635.44	Joback Method
cpg	559.17	J/mol×K	793.48	Joback Method
cpg	549.17	J/mol×K	767.14	Joback Method
cpg	538.73	J/mol×K	740.80	Joback Method
cpg	527.84	J/mol×K	714.46	Joback Method
cpg	516.48	J/mol×K	688.12	Joback Method
cpg	504.64	J/mol×K	661.78	Joback Method
dvisc	0.0002230	Pa×s	485.40	Joback Method
dvisc	0.0000217	Pa×s	635.44	Joback Method
dvisc	0.0000414	Pa×s	585.43	Joback Method
dvisc	0.0000888	Pa×s	535.42	Joback Method
dvisc	0.0183533	Pa×s	335.37	Joback Method
dvisc	0.0006920	Pa×s	435.39	Joback Method
dvisc	0.0028809	Pa×s	385.38	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.17069e+01
Coeff. B	-7.53576e+03
Coeff. C	-1.04100e+02
Temperature range (K), min.	455.92
Temperature range (K), max.	563.72

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765048&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect:	https://www.doi.org/10.1016/j.jct.2013.08.019

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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