

1,2-Decanediol

Other names:	decane-1,2-diol
Inchi:	InChI=1S/C10H22O2/c1-2-3-4-5-6-7-8-10(12)9-11/h10-12H,2-9H2,1H3
InchiKey:	YRSBDQINUMTIF-UHFFFAOYSA-N
Formula:	C10H22O2
SMILES:	CCCCCCCC(O)CO
Mol. weight [g/mol]:	174.28
CAS:	1119-86-4

Physical Properties

Property code	Value	Unit	Source
gf	-242.76	kJ/mol	Joback Method
hf	-559.47	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	70.82	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.090		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1419.00		NIST Webbook
tb	528.20	K	NIST Webbook
tc	771.40	K	Joback Method
tf	321.65 ± 0.30	K	NIST Webbook
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.00	J/molxK	612.12	Joback Method
cpg	453.83	J/molxK	638.67	Joback Method
cpg	465.19	J/molxK	665.21	Joback Method
cpg	476.08	J/molxK	691.76	Joback Method
cpg	486.52	J/molxK	718.31	Joback Method
cpg	496.52	J/molxK	744.85	Joback Method
cpg	506.10	J/molxK	771.40	Joback Method

dvisc	0.0507965	Paxs	309.10	Joback Method
dvisc	0.0059248	Paxs	359.60	Joback Method
dvisc	0.0011731	Paxs	410.11	Joback Method
dvisc	0.0003313	Paxs	460.61	Joback Method
dvisc	0.0001201	Paxs	511.11	Joback Method
dvisc	0.0000523	Paxs	561.62	Joback Method
dvisc	0.0000261	Paxs	612.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.81961e+01
Coeff. B	-5.99207e+03
Coeff. C	-9.49260e+01
Temperature range (K), min.	429.52
Temperature range (K), max.	559.98

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1119864&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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