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: YSRSBDQINUMTIF-UHFFFAOYSA-N
Formula: C10H22O2
SMILES: CCCCCCCCC(O)CO
Mol. weight [g/mol]: 174.28
CAS: 1119-86-4

Physical Properties

Property code	Value	Unit	Source
af	0.8730		Cheméo Relay (1.0)
gf	-242.76	kJ/mol	Joback Method
hf	-565.29	kJ/mol	Cheméo Relay (1.0)
hfus	26.31	kJ/mol	Joback Method
hvap	101.92	kJ/mol	Cheméo Relay (1.0)
ie	9.99	eV	Cheméo Relay (1.0)
log10ws	-2.44		Cheméo Relay (1.0)
logp	2.090		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
tb	549.83	K	Cheméo Relay (1.0)
tc	730.06	K	Cheméo Relay (1.0)
tf	322.24	K	Cheméo Relay (1.0)
vc	0.625	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	506.10	J/mol×K	771.40	Joback Method
dvisc	0.0507965	Pa×s	309.10	Joback Method
dvisc	0.0059248	Pa×s	359.60	Joback Method
dvisc	0.0011731	Pa×s	410.11	Joback Method
dvisc	0.0003313	Pa×s	460.61	Joback Method
dvisc	0.0001201	Pa×s	511.11	Joback Method
dvisc	0.0000523	Pa×s	561.62	Joback Method
dvisc	0.0000261	Pa×s	612.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119864&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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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

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