

1-Decanol, 2,2-dimethyl-

Other names:	1-Hydroxy-2,2-dimethyldecane 2,2-Dimethyl-1-decanol
Inchi:	InChI=1S/C12H26O/c1-4-5-6-7-8-9-10-12(2,3)11-13/h13H,4-11H2,1-3H3
InchiKey:	OSJLCOMCKUOKDD-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CCCCCCCC(C)(C)CO
Mol. weight [g/mol]:	186.33
CAS:	2370-15-2

Physical Properties

Property code	Value	Unit	Source
gf	-83.82	kJ/mol	Joback Method
hf	-451.99	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.756		Crippen Method
mvol	185.810	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
ripol	1911.00		NIST Webbook
ripol	1911.00		NIST Webbook
tb	517.15 ± 4.00	K	NIST Webbook
tc	727.78	K	Joback Method
tf	288.24	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.31	J/molxK	562.91	Joback Method
cpg	551.37	J/molxK	700.30	Joback Method
cpg	538.62	J/molxK	672.83	Joback Method
cpg	525.27	J/molxK	645.35	Joback Method
cpg	511.28	J/molxK	617.87	Joback Method

cpg	496.64	J/molxK	590.39	Joback Method
cpg	563.54	J/molxK	727.78	Joback Method
dvisc	0.0000801	Paxs	562.91	Joback Method
dvisc	0.0001367	Paxs	517.13	Joback Method
dvisc	0.0002589	Paxs	471.35	Joback Method
dvisc	0.0005625	Paxs	425.57	Joback Method
dvisc	0.0014737	Paxs	379.80	Joback Method
dvisc	0.0050272	Paxs	334.02	Joback Method
dvisc	0.0253239	Paxs	288.24	Joback Method

Sources

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=C2370152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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