

4-Decanol

Other names:	1-Propylheptyl alcohol Decanol-4 decan-4-ol
Inchi:	InChI=1S/C10H22O/c1-3-5-6-7-9-10(11)8-4-2/h10-11H,3-9H2,1-2H3
InchiKey:	DTDMYWXTWWFLGJ-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCCCCC(O)CCC
Mol. weight [g/mol]:	158.28
CAS:	2051-31-2

Physical Properties

Property code	Value	Unit	Source
gf	-105.94	kJ/mol	Joback Method
hf	-407.24	kJ/mol	Joback Method
hfus	22.22	kJ/mol	Joback Method
hvap	54.14	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.118		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rhoc	245.34 ± 6.33	kg/m ³	NIST Webbook
rhoc	245.34	kg/m ³	NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1544.00		NIST Webbook
ripol	1545.00		NIST Webbook
tb	483.70	K	NIST Webbook
tc	664.00 ± 1.00	K	NIST Webbook
tc	663.70	K	NIST Webbook
tc	633.72 ± 0.30	K	NIST Webbook
tf	248.28	K	Joback Method
vc	0.643	m ³ /kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.84	J/molxK	519.94	Joback Method
cpg	443.35	J/molxK	654.37	Joback Method
cpg	431.84	J/molxK	627.48	Joback Method
cpg	419.85	J/molxK	600.60	Joback Method
cpg	407.36	J/molxK	573.71	Joback Method
cpg	394.36	J/molxK	546.83	Joback Method
cpg	454.40	J/molxK	681.25	Joback Method
dvisc	0.0001173	Paxs	519.94	Joback Method
dvisc	0.0002038	Paxs	474.66	Joback Method
dvisc	0.0003977	Paxs	429.39	Joback Method
dvisc	0.0009085	Paxs	384.11	Joback Method
dvisc	0.0025882	Paxs	338.83	Joback Method
dvisc	0.0101842	Paxs	293.56	Joback Method
dvisc	0.0660457	Paxs	248.28	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63336e+01
Coeff. B	-4.78259e+03
Coeff. C	-7.54660e+01
Temperature range (K), min.	373.52
Temperature range (K), max.	509.37

Sources

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=C2051312&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
rhoc:	Critical density
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

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