3-Decanol

Inchi: InChI=1S/C10H22O/c1-3-5-6-7-8-9-10(11)4-2/h10-11H,3-9H2,1-2H3
InchiKey: ICEQLCZWZXUUIJ-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CCCCCCCC(O)CC
Mol. weight [g/mol]: 158.28
CAS: 1565-81-7

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	kg/m3	NIST Webbook
rhoc	245.34 ± 6.33	kg/m3	NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1189.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1602.00		NIST Webbook
tb	519.94	K	Joback Method
tc	666.00 ± 1.00	K	NIST Webbook
tc	666.10	K	NIST Webbook
tc	666.11 ± 0.30	K	NIST Webbook
tf	248.28	K	Joback Method
vc	0.643	m3/kmol	NIST Webbook

Temperature Dependent Properties

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60231e+01
Coeff. B	-4.68879e+03
Coeff. C	-7.54240e+01
Temperature range (K), min.	373.40
Temperature range (K), max.	513.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1565817&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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