1-Octanol, 2-butyl-

Other names:	2-Butyl-1-octanol
	2-Butyloctanol
	2-Butyloctyl alcohol
	2-butyloctan-1-ol
	5-(Hydroxymethyl)undecane
	Isododecyl alcohol
	Michel XO-150-12
Inchi:	InChI=1S/C12H26O/c1-3-5-7-8-10-12(11-13)9-6-4-2/h12-13H,3-11H2,1-2H3
InchiKey:	XMVBHZBLHNOQON-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CCCCCCC(CO)CCCC
Mol. weight [g/mol]:	186.33
CAS:	3913-02-8

Physical Properties

Property code	Value	Unit	Source
gf	-89.10	kJ/mol	Joback Method
hf	-448.52	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.756		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1848.00		NIST Webbook
tb	565.70	K	Joback Method
tc	725.92	K	Joback Method
tf	270.82	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.62	J/mol×K	725.92	Joback Method
cpg	493.60	J/mol×K	592.40	Joback Method
cpg	507.92	J/mol×K	619.11	Joback Method
cpg	521.66	J/mol×K	645.81	Joback Method
cpg	534.85	J/mol×K	672.51	Joback Method
cpg	547.50	J/mol×K	699.22	Joback Method
cpg	478.70	J/mol×K	565.70	Joback Method
dvisc	0.0381702	Pa×s	270.82	Joback Method
dvisc	0.0062239	Pa×s	319.97	Joback Method
dvisc	0.0016449	Pa×s	369.11	Joback Method
dvisc	0.0005944	Pa×s	418.26	Joback Method
dvisc	0.0002660	Pa×s	467.41	Joback Method
dvisc	0.0000810	Pa×s	565.70	Joback Method
dvisc	0.0001387	Pa×s	516.55	Joback Method
pvap	1.12e-03	kPa	308.10	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	1.95e-03	kPa	312.90	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	3.25e-03	kPa	317.80	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	5.26e-03	kPa	322.70	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	8.24e-03	kPa	327.60	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction

pvap	0.01	kPa	332.50	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.02	kPa	337.50	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.03	kPa	342.60	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.05	kPa	347.60	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.07	kPa	352.60	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59414e+01
Coeff. B	-4.96393e+03
Coeff. C	-8.56130e+01
Temperature range (K), min.	402.72
Temperature range (K), max.	552.59

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=C3913028&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
Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction:	https://www.doi.org/10.1021/acs.jced.9b00419

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
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