2,2,3,3,4,4,4-Heptafluoro-butanol

Other names:	1,1-Dihydroperfluorobutanol
	1,1-Dihydroperfluorobutyl alcohol
	1,1-H,H-Heptafluorobutanol
	1,1H-perfluorobutanol
	1-Butanol, 2,2,3,3,4,4,4-heptafluoro-
	1H,1H-Heptafluoro-1-butanol
	1H,1H-Heptafluorobutanol-1
	2,2,3,3,4,4,4-Heptafluoro-1-butanol
	2,2,3,3,4,4,4-heptafluorobutan-1-ol
	2,2,3,3,4,4,4-heptafluorobutanol
	Butanol, 2,2,3,3,4,4,4-heptafluoro-
	NSC 60528
	Perfluoro-1,1-dihydrobutanol
	«alpha»,«alpha»-Dihydroperfluorobutanol
	Â«alphaÂ»,Â«alphaÂ»-Dihydroperfluorobutanol
Inchi:	InChI=1S/C4H3F7O/c5-2(6,1-12)3(7,8)4(9,10)11/h12H,1H2
InchiKey:	WXJFKAZDSQLPBX-UHFFFAOYSA-N
Formula:	C4H3F7O
SMILES:	OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	200.05
CAS:	375-01-9

Physical Properties

Property code	Value	Unit	Source
chl	-1474.00 ± 6.30	kJ/mol	NIST Webbook
gf	-1509.17	kJ/mol	Joback Method
hf	-1677.14	kJ/mol	Joback Method
hfl	-1781.90 ± 6.30	kJ/mol	NIST Webbook
hfus	9.52	kJ/mol	Joback Method
hvap	31.57	kJ/mol	Joback Method
ie	11.20	eV	NIST Webbook
log10ws	-2.05		Crippen Method
logp	1.812		Crippen Method
mcvol	85.480	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
tb	368.20	K	NIST Webbook
tb	369.50 ± 0.50	K	NIST Webbook

tb	369.70	K	NIST Webbook
tb	368.80 ± 0.80	K	NIST Webbook
tc	503.34	K	Joback Method
tf	207.05	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.20	J/mol×K	368.30	Joback Method
cpg	204.29	J/mol×K	390.81	Joback Method
cpg	211.87	J/mol×K	413.31	Joback Method
cpg	218.96	J/mol×K	435.82	Joback Method
cpg	225.59	J/mol×K	458.32	Joback Method
cpg	231.77	J/mol×K	480.83	Joback Method
cpg	237.53	J/mol×K	503.34	Joback Method
hvapt	48.30	kJ/mol	303.05	Vapor pressure and liquid density of fluorinated alcohols: experimental, simulation and GC-SAFT-VR predictions
hvapt	43.60	kJ/mol	285.50	NIST Webbook
rhol	1580.00	kg/m3	293.15	Isothermal Vapor-Liquid Equilibrium Data for the Binary Systems Consisting of 1,1,2,3,3,3-Hexafluoro-1-propene and Either Methylcyclohexane, Cyclohexane, n-Hexane, 2-Methyltetrahydrofuran, or 2,2,3,3,4,4,4-Heptafluoro-1-butanol

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.88598e+01
Coeff. B	-5.24299e+03
Temperature range (K), min.	273.00
Temperature range (K), max.	386.99

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C375019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Fluorinated surfactants in solution:	https://www.doi.org/10.1016/j.fluid.2015.06.006
Diffusion coefficients of fluorinated alcohols in water:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
The Yaws Handbook of Vapor Pressure:	https://www.doi.org/10.1016/j.fluid.2016.06.011
Vapor pressure and liquid density of fluorinated alcohols: experimental, simulation and GC-SAFT-VR predictions.	https://www.doi.org/10.1021/acs.jced.9b00441
Isothermal Vapor-Liquid Equilibrium Data for the Binary Systems Consisting of 1,1,2,3,3,3-Hexafluoro-1-propene and Either Methylcyclohexane, Cyclohexane, n-Hexane, 2-Methyltetrahydrofuran, or 2,2,3,3,4,4,4-Heptafluoro-1-butanol:	

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume