Perfluorooctyl bromide

Other names:	1-Bromoperfluorooctane
	1-bromoheptadecafluorooctane
Inchi:	InChI=1S/C8BrF17/c9-7(22,23)5(18,19)3(14,15)1(10,11)2(12,13)4(16,17)6(20,21)8(24,25
InchiKey:	WTWWXOGTJWMJHI-UHFFFAOYSA-N
Formula:	C8BrF17
SMILES:	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br
Mol. weight [g/mol]:	498.96
CAS:	423-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-3258.25	kJ/mol	Joback Method
hf	-3585.99	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	45.60 ± 0.40	kJ/mol	NIST Webbook
log10ws	-6.96		Crippen Method
logp	6.348		Crippen Method
mcvol	171.170	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
tb	410.35	K	Joback Method
tc	536.18	K	Joback Method
tf	269.11	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.77	J/mol×K	410.35	Joback Method
cpg	456.22	J/mol×K	452.29	Joback Method
cpg	467.52	J/mol×K	473.26	Joback Method
cpg	477.92	J/mol×K	494.24	Joback Method
cpg	487.48	J/mol×K	515.21	Joback Method
cpg	496.22	J/mol×K	536.18	Joback Method
cpg	443.99	J/mol×K	431.32	Joback Method

hfust	12.13	kJ/mol	278.90	NIST Webbook
hfust	12.13	kJ/mol	278.90	NIST Webbook
hfust	1.60	kJ/mol	146.40	NIST Webbook
kvisc	0.0000008	m2/s	318.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000008	m2/s	313.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000009	m2/s	308.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000011	m2/s	298.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000010	m2/s	303.15	Viscosities of Liquid Fluorocompounds
pvap	2.24	kPa	318.09	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	4.70	kPa	332.78	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	1.67	kPa	313.18	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	1.30	kPa	308.22	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	0.98	kPa	303.26	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	3.69	kPa	327.88	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	0.69	kPa	298.08	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	0.54	kPa	293.20	Densities and Vapor Pressures of Highly Fluorinated Compounds

pvap	2.89	kPa	322.92	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	0.38	kPa	288.22	Densities and Vapor Pressures of Highly Fluorinated Compounds
rhol	1869.53	kg/m3	311.72	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhol	1926.65	kg/m3	288.63	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhol	1917.00	kg/m3	292.57	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhol	1906.56	kg/m3	298.78	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhol	1892.19	kg/m3	302.71	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids

rhol	1881.37	kg/m3	307.01	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
sfust	43.49	J/mol×K	278.90	NIST Webbook
sfust	10.93	J/mol×K	146.40	NIST Webbook
srf	0.02	N/m	318.55	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	287.15	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	292.75	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	303.35	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	308.45	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	313.45	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	298.35	Surface Tension of Liquid Fluorocompounds

Sources

Viscosities of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je700632z
liquid-liquid equilibrium of substituted perfluoro-n-octane + n-octane systems:	https://www.doi.org/10.1016/j.fluid.2008.04.011
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of oxygen in substituted perfluorocarbons:	https://www.doi.org/10.1016/j.fluid.2005.09.011
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Densities and Vapor Pressures of Highly Fluorinated Compounds:	https://www.doi.org/10.1021/je050056e
Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids:	https://www.doi.org/10.1016/j.jct.2006.11.012
Surface Tension of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je060199g
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C423552&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
kvisc:	Kinematic viscosity
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
sfust:	Entropy of fusion at a given temperature
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume