

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)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	456.22	J/molxK	452.29	Joback Method
cpg	443.99	J/molxK	431.32	Joback Method
cpg	496.22	J/molxK	536.18	Joback Method
cpg	487.48	J/molxK	515.21	Joback Method
cpg	477.92	J/molxK	494.24	Joback Method
cpg	467.52	J/molxK	473.26	Joback Method
cpg	430.77	J/molxK	410.35	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	0.0000011	m2/s	298.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000008	m2/s	313.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000008	m2/s	318.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000010	m2/s	303.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000009	m2/s	308.15	Viscosities of Liquid Fluorocompounds
pvap	0.54	kPa	293.20	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	0.69	kPa	298.08	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	0.38	kPa	288.22	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	1.30	kPa	308.22	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	1.67	kPa	313.18	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	2.24	kPa	318.09	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	2.89	kPa	322.92	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	3.69	kPa	327.88	Densities and Vapor Pressures of Highly Fluorinated Compounds

pvap	0.98	kPa	303.26	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	4.70	kPa	332.78	Densities and Vapor Pressures of Highly Fluorinated Compounds
rhoI	1926.65	kg/m3	288.63	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhoI	1917.00	kg/m3	292.57	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhoI	1906.56	kg/m3	298.78	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhoI	1892.19	kg/m3	302.71	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhoI	1881.37	kg/m3	307.01	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids

rhoI	1869.53	kg/m3	311.72	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
sfust	10.93	J/molxK	146.40	NIST Webbook
sfust	43.49	J/molxK	278.90	NIST Webbook
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	298.35	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	318.55	Surface Tension of Liquid Fluorocompounds

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C423552&Units=SI>

liquid-liquid equilibrium of substituted perfluoro-n-octane + n-octane systems:
Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids:
Solubility of oxygen in substituted perfluorocarbons:
McGowan Method:

<https://www.doi.org/10.1016/j.fluid.2008.04.011>

<https://www.doi.org/10.1016/j.jct.2006.11.012>

https://en.wikipedia.org/wiki/Joback_method

<https://www.doi.org/10.1016/j.fluid.2005.09.011>

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Surface Tension of Liquid Fluorocompounds:
Densities and Vapor Pressures of Highly Fluorinated Compounds:
Viscosities of Liquid Fluorocompounds:
Crippen Method:

<https://www.doi.org/10.1021/je060199g>

<https://www.doi.org/10.1021/je050056e>

<https://www.doi.org/10.1021/je700632z>

https://www.chemeo.com/doc/models/crippen_log10ws

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
rho:	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

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