1H-Perfluorooctane

Other names: 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluorooctane
octane, 1H-heptadecafluoro-
Inchi: InChI=1S/C8HF17/c9-1(10)2(11,12)3(13,14)4(15,16)5(17,18)6(19,20)7(21,22)8(23,24)25
InchiKey: KBHBUUBXEQUIMV-UHFFFAOYSA-N
Formula: C8HF17
SMILES: FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 420.07
CAS: 335-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-3277.85	kJ/mol	Joback Method
hf	-3608.85	kJ/mol	Joback Method
hfus	13.41	kJ/mol	Joback Method
hvap	43.40 ± 0.20	kJ/mol	NIST Webbook
log10ws	-6.03		Crippen Method
logp	5.626		Crippen Method
mcvol	153.670	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinpol	395.00		NIST Webbook
tb	346.98	K	Joback Method
tc	454.35	K	Joback Method
tf	191.89	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.70	J/mol×K	454.35	Joback Method
cpg	429.53	J/mol×K	436.46	Joback Method
cpg	418.73	J/mol×K	418.56	Joback Method
cpg	407.26	J/mol×K	400.67	Joback Method
cpg	395.10	J/mol×K	382.77	Joback Method
cpg	382.23	J/mol×K	364.88	Joback Method

cpg	368.62	J/mol×K	346.98	Joback Method
pvap	10.25	kPa	328.00	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	8.07	kPa	323.01	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	12.83	kPa	332.89	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	6.22	kPa	318.06	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	4.87	kPa	313.13	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	3.72	kPa	308.15	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	2.84	kPa	303.19	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	2.18	kPa	298.26	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	1.60	kPa	293.26	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	1.18	kPa	288.35	Densities and Vapor Pressures of Highly Fluorinated Compounds

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C335659&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
liquid-liquid equilibrium of substituted perfluoro-n-octane + n-octane systems:	https://www.doi.org/10.1016/j.fluid.2008.04.011
Densities and Vapor Pressures of Highly Fluorinated Compounds:	https://www.doi.org/10.1021/je050056e
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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