

Pentadecafluorooctanoic acid

Other names:	2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Pentadecafluorooctanoic acid 65618-66-8 71244-15-0 Fluorad FC-26 Hexanoyl fluoride, 3,3,4,4,5,5,6,6,6-nonafluoro-2-oxo- NSC 95114 Octanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro- Octanoic acid, pentadecafluoro- PFOA Pentadecafluoro-1-octanoic acid Pentadecafluoro-n-octanoic acid Perfluoro-n-octanoic acid Perfluorocaprylic acid Perfluorooctanoic acid Perfluoroheptanecarboxylic acid Perfluorooctanoic acid n-Perfluorooctanoic acid
Inchi:	InChI=1S/C8HF15O2/c9-2(10,1(24)25)3(11,12)4(13,14)5(15,16)6(17,18)7(19,20)8(21,22
InchiKey:	SNGREZUHAYWORS-UHFFFAOYSA-N
Formula:	C8HF15O2
SMILES:	O=C(O)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]:	414.07
CAS:	335-67-1

Physical Properties

Property code	Value	Unit	Source
gf	-3151.53	kJ/mol	Joback Method
hf	-3476.16	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	35.50	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.445		Crippen Method
mcvol	157.570	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	1045.00		NIST Webbook
rinpol	1045.00		NIST Webbook
tb	494.93	K	Joback Method

tc	624.79	K	Joback Method
tf	316.46	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.33	J/mol×K	624.79	Joback Method
cpg	497.07	J/mol×K	603.14	Joback Method
cpg	490.20	J/mol×K	581.50	Joback Method
cpg	482.67	J/mol×K	559.86	Joback Method
cpg	474.45	J/mol×K	538.22	Joback Method
cpg	465.49	J/mol×K	516.57	Joback Method
cpg	455.75	J/mol×K	494.93	Joback Method
hsubt	88.90	kJ/mol	308.00	NIST Webbook
psub	0.04	kPa	318.85	Solid Vapor Pressure and Enthalpy of Sublimation for Perfluorooctanoic Acid
psub	5.20e-03	kPa	294.85	Solid Vapor Pressure and Enthalpy of Sublimation for Perfluorooctanoic Acid
psub	0.02	kPa	308.55	Solid Vapor Pressure and Enthalpy of Sublimation for Perfluorooctanoic Acid
pvap	0.58	kPa	352.15	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	4.59	kPa	387.15	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids

pvap	0.36	kPa	345.75	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	13.07	kPa	409.26	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	22.16	kPa	421.75	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	37.25	kPa	435.35	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	63.98	kPa	450.95	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	96.50	kPa	463.95	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	0.23	kPa	339.75	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids

pvap	0.17	kPa	335.52	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	0.13	kPa	332.40	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	2.69	kPa	377.09	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	1.60	kPa	368.05	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	0.96	kPa	359.75	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	7.69	kPa	397.55	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	462.20	K	98.10	NIST Webbook
tbrp	462.00	K	98.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C335671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids:	https://www.doi.org/10.1021/je050070r
Solid Vapor Pressure and Enthalpy of Sublimation for Perfluorooctanoic Acid:	https://www.doi.org/10.1021/je700593d
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
hsubt:	Enthalpy of sublimation at a given temperature
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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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