Perfluorononanoic acid

Other names:	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-Heptadecafluorononanoic acid
	Nonanoic acid, heptadecafluoro-
	perfluorononan-1-oic acid
Inchi:	InChI=1S/C9HF17O2/c10-2(11,1(27)28)3(12,13)4(14,15)5(16,17)6(18,19)7(20,21)8(22,2
InchiKey:	UZUFPBIDKMEQEQ-UHFFFAOYSA-N
Formula:	C9HF17O2
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)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	464.08
CAS:	375-95-1

Physical Properties

Property code	Value	Unit	Source
gf	-3529.89	kJ/mol	Joback Method
hf	-3897.77	kJ/mol	Joback Method
hfus	17.80	kJ/mol	Joback Method
hvap	34.80	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.080		Crippen Method
mcvol	175.200	ml/mol	McGowan Method
pc	1550.00	kPa	Joback Method
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook
tb	513.12	K	Joback Method
tc	641.08	K	Joback Method
tf	331.33	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.84	J/mol×K	513.12	Joback Method
cpg	530.88	J/mol×K	534.45	Joback Method
cpg	540.11	J/mol×K	555.77	Joback Method
cpg	548.57	J/mol×K	577.10	Joback Method

cpg	556.29	J/mol×K	598.43	Joback Method
cpg	563.33	J/mol×K	619.76	Joback Method
cpg	569.73	J/mol×K	641.08	Joback Method
pvap	3.12	kPa	390.81	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	2.02	kPa	382.69	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	1.12	kPa	372.78	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	5.54	kPa	401.70	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	9.33	kPa	412.92	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	15.19	kPa	423.86	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	22.77	kPa	432.85	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids

pvap	37.25	kPa	446.11	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	62.07	kPa	461.08	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	99.97	kPa	476.13	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	99.97	kPa	476.27	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C375951&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
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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