

Dodecanoic acid, tricosafuoro-

Other names:	Perfluorododecanoic acid tricosafuorododecanoic acid
Inchi:	InChI=1S/C12HF23O2/c13-2(14,1(36)37)3(15,16)4(17,18)5(19,20)6(21,22)7(23,24)8(25,
InchiKey:	CXGONMQFMIYUJR-UHFFFAOYSA-N
Formula:	C ₁₂ H _F ₂₃ O ₂
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)C(F)(F)C(F)(F)C(F)(F)
Mol. weight [g/mol]:	614.10
CAS:	307-55-1

Physical Properties

Property code	Value	Unit	Source
gf	-4664.97	kJ/mol	Joback Method
hf	-5162.60	kJ/mol	Joback Method
hfus	21.81	kJ/mol	Joback Method
hvap	32.68	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.986		Crippen Method
mcvol	228.090	ml/mol	McGowan Method
pc	1081.35	kPa	Joback Method
tb	567.69	K	Joback Method
tc	696.47	K	Joback Method
tf	375.94	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.30	J/mol×K	567.69	Joback Method
cpg	733.97	J/mol×K	589.15	Joback Method
cpg	743.68	J/mol×K	610.62	Joback Method
cpg	752.48	J/mol×K	632.08	Joback Method
cpg	760.45	J/mol×K	653.55	Joback Method
cpg	767.63	J/mol×K	675.01	Joback Method
cpg	774.10	J/mol×K	696.47	Joback Method

pvap	2.85	kPa	422.10	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	1.82	kPa	413.72	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	0.86	kPa	400.73	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	2.98	kPa	422.75	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	4.85	kPa	433.27	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	8.29	kPa	445.63	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	13.81	kPa	457.94	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids

pvap	22.07	kPa	470.59	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	34.48	kPa	483.66	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	55.15	kPa	498.85	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids
pvap	99.96	kPa	520.51	Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C307551&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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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