

1-Octanol, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-

Other names: (perfluoroheptyl)methanol
1,1-dihydroperfluorooctanol
1,1H-perfluorooctanol
1H,1H-Pentadecafluoro-1-octanol
1H,1H-Pentadecafluorooctanol
1H,1H-Pentadecafluorooctanol-1
1H,1H-Perfluoro-1-octanol
1H,1H-Perfluorooctanol
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Pentadecafluoro-1-octanol
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Pentadecafluorooctyl alcohol
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctan-1-ol
Caprylic alcohol, pentadecafluoro-
Pentadecafluorocaprylic alcohol
Pentadecafluorooctyl alcohol

Inchi: InChI=1S/C8H3F15O/c9-2(10,1-24)3(11,12)4(13,14)5(15,16)6(17,18)7(19,20)8(21,22)23

InchiKey: PJDOLCGOTSNFJM-UHFFFAOYSA-N

Formula: C8H3F15O

SMILES: OCC(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]: 400.08

CAS: 307-30-2

Physical Properties

Property code	Value	Unit	Source
gf	-3022.61	kJ/mol	Joback Method
hf	-3363.58	kJ/mol	Joback Method
hfus	11.90	kJ/mol	Evidence of an odd-even effect on the thermodynamic parameters of odd fluorotelomer alcohols
hvap	28.75	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.353		Crippen Method
mcvol	156.000	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
tb	437.20	K	NIST Webbook
tb	419.00	K	NIST Webbook
tc	561.29	K	Joback Method

tf	266.53	K	Joback Method
vc	0.696	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.40	J/mol×K	541.25	Joback Method
cpg	430.00	J/mol×K	441.06	Joback Method
cpg	441.33	J/mol×K	461.10	Joback Method
cpg	451.91	J/mol×K	481.14	Joback Method
cpg	461.76	J/mol×K	501.18	Joback Method
cpg	470.91	J/mol×K	521.21	Joback Method
cpg	487.26	J/mol×K	561.29	Joback Method
hvapt	53.30	kJ/mol	393.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.93403e+01
Coeff. B	-6.43573e+03
Temperature range (K), min.	337.78
Temperature range (K), max.	458.75

Sources

Evidence of an odd-even effect on the thermodynamic parameters of odd-numbered alcohols:	https://www.doi.org/10.1016/j.jct.2012.03.027
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C307302&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	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
hvac:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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