

1H,1H,7H-Dodecafluoro-1-heptanol

Other names:	1,1,7-Trihydrododecafluoroheptan-1-ol 1,1,7-Trihydrododecafluoroheptanol 1,1,7-Trihydroperfluoroheptanol 1,1,7-Trihydroperfluoroheptyl alcohol 1,1,7H-perfluoroheptanol 1-Heptanol, 1H,1H,7H-dodecafluoro- 1-Heptanol, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro- 1H,1H,7H-Dodecafluoro-1-hydroxyheptane 1H,1H,7H-Dodecafluoroheptanol 1H,1H,7H-Perfluoroheptanol 2,2,3,3,4,4,5,5,6,6,7,7-Dodecafluoro-1-heptanol 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptan-1-ol NSC 115
Inchi:	InChI=1S/C7H4F12O/c8-2(9)4(12,13)6(16,17)7(18,19)5(14,15)3(10,11)1-20/h2,20H,1H2
InchiKey:	BYKNGMLDSIEFFG-UHFFFAOYSA-N
Formula:	C7H4F12O
SMILES:	OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]:	332.09
CAS:	335-99-9

Physical Properties

Property code	Value	Unit	Source
gf	-2454.72	kJ/mol	Joback Method
hf	-2742.39	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	31.18	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.420		Crippen Method
mcvol	136.600	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	868.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	868.00		NIST Webbook
tb	442.50 ± 0.50	K	NIST Webbook
tc	550.75	K	Joback Method
tf	233.65	K	Joback Method

vc	0.602	m3/kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.74	J/mol×K	550.75	Joback Method
cpg	404.25	J/mol×K	530.02	Joback Method
cpg	396.21	J/mol×K	509.29	Joback Method
cpg	387.60	J/mol×K	488.57	Joback Method
cpg	378.39	J/mol×K	467.84	Joback Method
cpg	368.54	J/mol×K	447.12	Joback Method
cpg	358.04	J/mol×K	426.39	Joback Method
hvapt	53.40	kJ/mol	400.50	NIST Webbook
rho1	1678.50	kg/m3	333.15	Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures
rho1	1696.90	kg/m3	323.15	Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures
rho1	1715.00	kg/m3	313.15	Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures
rho1	1732.70	kg/m3	303.15	Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures
rho1	1750.20	kg/m3	293.15	Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures
rho1	1750.10	kg/m3	293.15	Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures

rho	1659.70	kg/m ³	343.15	Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.91366e+01
Coeff. B	-6.42651e+03
Temperature range (K), min.	340.95
Temperature range (K), max.	464.84

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

Crippen Method:

Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures:

McGowan Method:

NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

<https://www.doi.org/10.1016/j.fluid.2006.10.025>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C335999&Units=SI>

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
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
rhoL:	Liquid Density
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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