1-Octanethiol

Other names:	1-Mercaptooctane
	1-Octyl mercaptan
	1-Octylthiol
	N-OCTYL MERCAPTAN
	NSC 41903
	OCTANE-1-THIOL
	OCTYLTHIOL
	Octanethiol-(1)
	Octyl mercaptan
	n-Octanethiol
	n-Octylthiol
Inchi:	InChI=1S/C8H18S/c1-2-3-4-5-6-7-8-9/h9H,2-8H2,1H3
InchiKey:	KZCOBXFFBQJQHH-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CCCCCCCCS
Mol. weight [g/mol]:	146.29
CAS:	111-88-6

Physical Properties

Property code	Value	Unit	Source
gf	45.87	kJ/mol	Joback Method
hf	-169.97	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	40.14	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.277		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1140.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1369.00		NIST Webbook
tb	472.30	K	NIST Webbook

tc	630.81	K	Joback Method
tf	224.00 ± 0.30	K	NIST Webbook
tf	224.00 ± 0.40	K	NIST Webbook
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.32	J/mol×K	599.89	Joback Method
cpg	284.69	J/mol×K	445.30	Joback Method
cpg	298.55	J/mol×K	476.22	Joback Method
cpg	311.83	J/mol×K	507.14	Joback Method
cpg	324.54	J/mol×K	538.06	Joback Method
cpg	336.70	J/mol×K	568.97	Joback Method
cpg	359.43	J/mol×K	630.81	Joback Method
cpl	300.24	J/mol×K	300.00	NIST Webbook
hfust	24.27	kJ/mol	224.00	NIST Webbook
hfust	24.27	kJ/mol	224.00	NIST Webbook
hvapt	49.60	kJ/mol	422.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53741e+01
Coeff. B	-4.31073e+03
Coeff. C	-7.24190e+01
Temperature range (K), min.	358.15
Temperature range (K), max.	500.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.14398e+02
Coeff. B	-1.06223e+04
Coeff. C	-1.44474e+01

Coeff. D	7.49591e-06
Temperature range (K), min.	223.95
Temperature range (K), max.	664.00

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1841
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111886&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1841
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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