1-Nonanethiol

Other names:	1-Nonylthiol
	NONYLTHIOL
	Nonyl mercaptan
	n-Nonyl mercaptan
	nonane-1-thiol
Inchi:	InChI=1S/C9H20S/c1-2-3-4-5-6-7-8-9-10/h10H,2-9H2,1H3
InchiKey:	ZVEZMVFBMOOHAT-UHFFFAOYSA-N
Formula:	C9H20S
SMILES:	CCCCCCCCCS
Mol. weight [g/mol]:	160.32
CAS:	1455-21-6

Physical Properties

Property code	Value	Unit	Source
gf	54.29	kJ/mol	Joback Method
hf	-190.61	kJ/mol	Joback Method
hfus	23.11	kJ/mol	Joback Method
hvap	42.37	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.667		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1218.00		NIST Webbook
ripol	1470.00		NIST Webbook
tb	493.20	K	NIST Webbook
tc	651.93	K	Joback Method
tf	253.10 ± 0.30	K	NIST Webbook
tf	253.10 ± 0.30	K	NIST Webbook
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.57	J/mol×K	560.05	Joback Method
cpg	383.59	J/mol×K	590.68	Joback Method
cpg	396.04	J/mol×K	621.30	Joback Method
cpg	327.87	J/mol×K	468.18	Joback Method
cpg	342.73	J/mol×K	498.80	Joback Method
cpg	356.96	J/mol×K	529.43	Joback Method
cpg	407.92	J/mol×K	651.93	Joback Method
hfust	33.50	kJ/mol	267.70	NIST Webbook
hfust	33.50	kJ/mol	267.70	NIST Webbook
hvapt	52.60	kJ/mol	442.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54623e+01
Coeff. B	-4.50037e+03
Coeff. C	-7.81900e+01
Temperature range (K), min.	374.76
Temperature range (K), max.	521.54

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.12426e+02
Coeff. B	-1.10877e+04
Coeff. C	-1.40128e+01
Coeff. D	6.43876e-06
Temperature range (K), min.	253.05
Temperature range (K), max.	681.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1455216&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=1845
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1845.mol

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
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