

2-nonanethiol

Inchi:	InChI=1S/C9H20S/c1-3-4-5-6-7-8-9(2)10/h9-10H,3-8H2,1-2H3
InchiKey:	UOMSUBPWUZCGQU-UHFFFAOYSA-N
Formula:	C9H20S
SMILES:	CCCCCCCC(C)S
Mol. weight [g/mol]:	160.32
CAS:	13281-11-3

Physical Properties

Property code	Value	Unit	Source
gf	51.85	kJ/mol	Joback Method
hf	-195.89	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	41.98	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.665		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
tb	467.74	K	Joback Method
tc	655.55	K	Joback Method
tf	204.20 ± 0.30	K	NIST Webbook
vc	0.588	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.99	J/mol×K	467.74	Joback Method
cpg	343.25	J/mol×K	499.04	Joback Method
cpg	357.86	J/mol×K	530.34	Joback Method
cpg	371.81	J/mol×K	561.64	Joback Method
cpg	385.13	J/mol×K	592.95	Joback Method
cpg	397.85	J/mol×K	624.25	Joback Method
cpg	409.97	J/mol×K	655.55	Joback Method
hvapt	50.30	kJ/mol	430.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47692e+01
Coeff. B	-4.20713e+03
Coeff. C	-7.49650e+01
Temperature range (K), min.	365.48
Temperature range (K), max.	519.80

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C13281113&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/ci9903071

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
mccvol:	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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