1,9-Nonanedithiol

Other names: 1,9-Dimercaptononane
nonane-1,9-dithiol
Inchi: InChI=1S/C9H20S2/c10-8-6-4-2-1-3-5-7-9-11/h10-11H,1-9H2
InchiKey: GJRCLMJHPWCJEI-UHFFFAOYSA-N
Formula: C9H20S2
SMILES: SCCCCCCCCCS
Mol. weight [g/mol]: 192.38
CAS: 3489-28-9

Physical Properties

Property code	Value	Unit	Source
gf	83.68	kJ/mol	Joback Method
hf	-152.13	kJ/mol	Joback Method
hfus	27.15	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.577		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
tb	531.04	K	Joback Method
tc	734.45	K	Joback Method
tf	264.11	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.59	J/mol×K	531.04	Joback Method
cpg	396.85	J/mol×K	564.94	Joback Method
cpg	411.36	J/mol×K	598.84	Joback Method
cpg	425.14	J/mol×K	632.74	Joback Method
cpg	438.21	J/mol×K	666.64	Joback Method
cpg	450.60	J/mol×K	700.55	Joback Method
cpg	462.34	J/mol×K	734.45	Joback Method

hvapt	63.60	kJ/mol	487.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37297e+01
Coeff. B	-4.33942e+03
Coeff. C	-9.52940e+01
Temperature range (K), min.	418.00
Temperature range (K), max.	610.77

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3489289&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume