Benzenepropanethiol

Other names:	1-Propanethiol, 3-phenyl-
	3-Phenyl-1-propanethiol
	3-Phenylpropanethiol
	3-Phenylpropyl mercaptan
	3-Phenylpropylthiol
	3-phenylpropane-1-thiol
	«gamma»-Phenylpropyl mercaptan
	Â«gammaÂ»-Phenylpropyl mercaptan
Inchi:	InChI=1S/C9H12S/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6,10H,4,7-8H2
InchiKey:	IUSDGVJFDZRIBR-UHFFFAOYSA-N
Formula:	C9H12S
SMILES:	SCCCc1ccccc1
Mol. weight [g/mol]:	152.26
CAS:	24734-68-7

Physical Properties

Property code	Value	Unit	Source
gf	166.70	kJ/mol	Joback Method
hf	45.92	kJ/mol	Joback Method
hfus	17.15	kJ/mol	Joback Method
hvap	44.64	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.549		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	494.86	K	Joback Method
tc	725.79	K	Joback Method
tf	254.07	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.34	J/mol×K	494.86	Joback Method

cpg	277.73	J/mol×K	533.35	Joback Method
cpg	291.18	J/mol×K	571.84	Joback Method
cpg	303.75	J/mol×K	610.32	Joback Method
cpg	315.46	J/mol×K	648.81	Joback Method
cpg	326.36	J/mol×K	687.30	Joback Method
cpg	336.50	J/mol×K	725.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41756e+01
Coeff. B	-4.08257e+03
Coeff. C	-8.07430e+01
Temperature range (K), min.	374.71
Temperature range (K), max.	541.31

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24734687&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume