Phenethyl mercaptan

Other names:	2-Phenylethanethiol
	2-Phenylethyl mercaptan
	2-Phenylethylthiol
	Benzeneethanethiol
	Phenylethylthiol
	«beta»-Phenylethyl mercaptan
	Â«betaÂ»-Phenylethyl mercaptan
Inchi:	InChI=1S/C8H10S/c9-7-6-8-4-2-1-3-5-8/h1-5,9H,6-7H2
InchiKey:	ZMRFRBHYXOQLDK-UHFFFAOYSA-N
Formula:	C8H10S
SMILES:	SCCc1ccccc1
Mol. weight [g/mol]:	138.23
CAS:	4410-99-5

Physical Properties

Property code	Value	Unit	Source
gf	158.28	kJ/mol	Joback Method
hf	66.56	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.159		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1147.00		NIST Webbook
tb	471.98	K	Joback Method
tc	707.00	K	Joback Method
tf	242.80	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.26	J/mol×K	471.98	Joback Method
cpg	234.52	J/mol×K	511.15	Joback Method
cpg	246.90	J/mol×K	550.32	Joback Method
cpg	258.43	J/mol×K	589.49	Joback Method
cpg	269.16	J/mol×K	628.66	Joback Method
cpg	279.13	J/mol×K	667.83	Joback Method
cpg	288.37	J/mol×K	707.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49598e+01
Coeff. B	-4.23248e+03
Coeff. C	-7.75510e+01
Temperature range (K), min.	366.02
Temperature range (K), max.	516.23

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4410995&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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