Benzenemethanethiol, «alpha»-methyl-

Other names:	1-Phenylethanethiol
	1-Phenylethyl mercaptane
Inchi:	InChI=1S/C8H10S/c1-7(9)8-5-3-2-4-6-8/h2-7,9H,1H3
InchiKey:	QZZBJCFNHPYNKO-UHFFFAOYSA-N
Formula:	C8H10S
SMILES:	CC(S)c1ccccc1
Mol. weight [g/mol]:	138.23
CAS:	6263-65-6

Physical Properties

Property code	Value	Unit	Source
gf	155.84	kJ/mol	Joback Method
hf	61.28	kJ/mol	Joback Method
hfus	11.04	kJ/mol	Joback Method
hvap	42.03	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.677		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
tb	471.54	K	Joback Method
tc	712.42	K	Joback Method
tf	227.80	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.45	J/mol×K	471.54	Joback Method
cpg	235.14	J/mol×K	511.69	Joback Method
cpg	247.88	J/mol×K	551.83	Joback Method
cpg	259.73	J/mol×K	591.98	Joback Method
cpg	270.72	J/mol×K	632.13	Joback Method

cpg	280.91	J/mol×K	672.27	Joback Method
cpg	290.33	J/mol×K	712.42	Joback Method

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=C6263656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume