1-Phenylethanethiol

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]: 138.24

Physical Properties

Property code	Value	Unit	Source
af	0.3443		Cheméo Relay (1.0)
gf	155.84	kJ/mol	Joback Method
hf	48.38	kJ/mol	Cheméo Relay (1.0)
hfus	11.04	kJ/mol	Joback Method
hvap	58.76	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-2.14		Cheméo Relay (1.0)
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	459.24	K	Cheméo Relay (1.0)
tc	696.91	K	Cheméo Relay (1.0)
tf	231.65	K	Cheméo Relay (1.0)
vc	0.410	m3/kmol	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6263656&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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