Benzenemethanethiol, «alpha»-phenyl-

Other names: Diphenylmethanethiol
Inchi: InChI=1S/C13H12S/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13-14H
InchiKey: ORKZATPRQQSLDT-UHFFFAOYSA-N
Formula: C13H12S
SMILES: SC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 200.30
CAS: 4237-48-3

Physical Properties

Property code	Value	Unit	Source
gf	310.35	kJ/mol	Joback Method
hf	190.00	kJ/mol	NIST Webbook
hfus	18.03	kJ/mol	Joback Method
hvap	55.43	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.706		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	612.62	K	Joback Method
tc	884.50	K	Joback Method
tf	310.57	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.43	J/mol×K	612.62	Joback Method
cpg	392.47	J/mol×K	657.93	Joback Method
cpg	407.95	J/mol×K	703.25	Joback Method
cpg	421.99	J/mol×K	748.56	Joback Method
cpg	434.70	J/mol×K	793.87	Joback Method
cpg	446.21	J/mol×K	839.18	Joback Method
cpg	456.60	J/mol×K	884.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4237483&Units=SI
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume