Mercapto-d1-benzene

Inchi: InChI=1S/C6H6S/c7-6-4-2-1-3-5-6/h1-5,7H/i/hD
InchiKey: RMVRSNDYEFQCLF-DYCDLGHISA-N
Formula: C6H5DS
SMILES: Sc1ccccc1
Mol. weight [g/mol]: 111.18
CAS: 15570-03-3

Physical Properties

Property code	Value	Unit	Source
gf	141.44	kJ/mol	Joback Method
hf	107.84	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	37.96	kJ/mol	Joback Method
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	1.975		Crippen Method
mcvol	87.990	ml/mol	McGowan Method
pc	5109.34	kPa	Joback Method
tb	426.22	K	Joback Method
tc	669.16	K	Joback Method
tf	220.26	K	Joback Method
vc	0.318	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.35	J/mol×K	426.22	Joback Method
cpg	153.83	J/mol×K	466.71	Joback Method
cpg	163.56	J/mol×K	507.20	Joback Method
cpg	172.58	J/mol×K	547.69	Joback Method
cpg	180.92	J/mol×K	588.18	Joback Method
cpg	188.62	J/mol×K	628.67	Joback Method
cpg	195.71	J/mol×K	669.16	Joback Method

Sources

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=C15570033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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