thiophenoxide anion

Inchi: InChI=1S/C6H6S/c7-6-4-2-1-3-5-6/h1-5,7H/p-1
InchiKey: RMVRSNDYEFQCLF-UHFFFAOYSA-M
Formula: C6H5S-
SMILES: [S-]c1ccccc1
Mol. weight [g/mol]: 109.17
CAS: 13133-62-5

Physical Properties

Property code	Value	Unit	Source
gf	197.55	kJ/mol	Joback Method
hf	167.04	kJ/mol	Joback Method
hfus	11.15	kJ/mol	Joback Method
hvap	37.90	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	1.592		Crippen Method
mcvol	85.840	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	431.44	K	Joback Method
tc	669.59	K	Joback Method
tf	234.57	K	Joback Method
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.43	J/mol×K	431.44	Joback Method
cpg	148.04	J/mol×K	471.13	Joback Method
cpg	156.82	J/mol×K	510.82	Joback Method
cpg	164.82	J/mol×K	550.52	Joback Method
cpg	172.11	J/mol×K	590.21	Joback Method
cpg	178.75	J/mol×K	629.90	Joback Method
cpg	184.80	J/mol×K	669.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13133625&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

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