Cyclopropyl phenyl sulphide

Other names: Cyclopropyl phenyl sulfide
Inchi: InChI=1S/C9H10S/c1-2-4-8(5-3-1)10-9-6-7-9/h1-5,9H,6-7H2
InchiKey: YIBKCPJOFAUAKY-UHFFFAOYSA-N
Formula: C9H10S
SMILES: c1ccc(SC2CC2)cc1
Mol. weight [g/mol]: 150.24
CAS: 14633-54-6

Physical Properties

Property code	Value	Unit	Source
gf	231.18	kJ/mol	Joback Method
hf	122.11	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	44.63	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.941		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	507.52	K	Joback Method
tc	757.45	K	Joback Method
tf	269.95	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.58	J/mol×K	507.52	Joback Method
cpg	266.06	J/mol×K	549.17	Joback Method
cpg	280.29	J/mol×K	590.83	Joback Method
cpg	293.36	J/mol×K	632.48	Joback Method
cpg	305.35	J/mol×K	674.14	Joback Method
cpg	316.36	J/mol×K	715.79	Joback Method
cpg	326.44	J/mol×K	757.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.70	K	0.10	NIST Webbook

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=C14633546&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume