Cyclohexyl phenyl sulfide

Inchi: InChI=1S/C12H16S/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1,3-4,7-8,12H,2,5-6,9-10H2
InchiKey: LWSWHXZQBIFYLZ-UHFFFAOYSA-N
Formula: C12H16S
SMILES: c1ccc(SC2CCCCC2)cc1
Mol. weight [g/mol]: 192.32
CAS: 7570-92-5

Physical Properties

Property code	Value	Unit	Source
gf	220.14	kJ/mol	Joback Method
hf	41.71	kJ/mol	Joback Method
hfus	16.84	kJ/mol	Joback Method
hvap	51.83	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.111		Crippen Method
mcvol	161.670	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	588.97	K	Joback Method
tc	850.96	K	Joback Method
tf	293.20	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.13	J/mol×K	588.97	Joback Method
cpg	414.12	J/mol×K	632.63	Joback Method
cpg	433.45	J/mol×K	676.30	Joback Method
cpg	451.18	J/mol×K	719.96	Joback Method
cpg	467.38	J/mol×K	763.63	Joback Method
cpg	482.13	J/mol×K	807.29	Joback Method
cpg	495.48	J/mol×K	850.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7570925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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