Sulfide, phenyl 3-phenylpropyl

Other names: Phenyl 3-phenylpropyl sulphide
Inchi: InChI=1S/C15H16S/c1-3-8-14(9-4-1)10-7-13-16-15-11-5-2-6-12-15/h1-6,8-9,11-12H,7,10
InchiKey: UJRJBPIWQWWQMB-UHFFFAOYSA-N
Formula: C15H16S
SMILES: c1ccc(CCCSc2ccccc2)cc1
Mol. weight [g/mol]: 228.35
CAS: 30134-12-4

Physical Properties

Property code	Value	Unit	Source
gf	333.36	kJ/mol	Joback Method
hf	162.00	kJ/mol	Joback Method
hfus	26.82	kJ/mol	Joback Method
hvap	60.35	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.412		Crippen Method
mcvol	191.040	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
tb	664.74	K	Joback Method
tc	917.12	K	Joback Method
tf	346.05	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.35	J/mol×K	664.74	Joback Method
cpg	495.91	J/mol×K	706.80	Joback Method
cpg	512.02	J/mol×K	748.87	Joback Method
cpg	526.77	J/mol×K	790.93	Joback Method
cpg	540.23	J/mol×K	832.99	Joback Method
cpg	552.50	J/mol×K	875.05	Joback Method
cpg	563.66	J/mol×K	917.12	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=C30134124&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