Benzene,[(4-phenoxybutyl)thio]-

Other names: 1-Phenoxy-4-phenylthio-butane
Inchi: InChI=1S/C16H18OS/c1-3-9-15(10-4-1)17-13-7-8-14-18-16-11-5-2-6-12-16/h1-6,9-12H,7
InchiKey: IEFUOVNESVMIQY-UHFFFAOYSA-N
Formula: C16H18OS
SMILES: c1ccc(OCCCCSc2ccccc2)cc1
Mol. weight [g/mol]: 258.38
CAS: 59950-11-7

Physical Properties

Property code	Value	Unit	Source
gf	236.78	kJ/mol	Joback Method
hf	9.14	kJ/mol	Joback Method
hfus	30.60	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
ie	8.25 ± 0.05	eV	NIST Webbook
log10ws	-4.82		Crippen Method
logp	4.638		Crippen Method
mcvol	211.000	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
tb	710.04	K	Joback Method
tc	952.82	K	Joback Method
tf	379.55	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.55	J/mol×K	710.04	Joback Method
cpg	574.82	J/mol×K	750.50	Joback Method
cpg	590.71	J/mol×K	790.97	Joback Method
cpg	605.26	J/mol×K	831.43	Joback Method
cpg	618.53	J/mol×K	871.90	Joback Method
cpg	630.59	J/mol×K	912.36	Joback Method
cpg	641.49	J/mol×K	952.82	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59950117&Units=SI

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