1-PHENOXY-4-PHENYLTHIO-BUTANE

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]: 258.39

Physical Properties

Property code	Value	Unit	Source
af	0.5900		Cheméo Relay (1.0)
hf	24.39	kJ/mol	Cheméo Relay (1.0)
hfus	30.60	kJ/mol	Joback Method
hvap	98.16	kJ/mol	Cheméo Relay (1.0)
ie	8.25 ± 0.05	eV	NIST Webbook
log10ws	-5.41		Cheméo Relay (1.0)
logp	4.638		Crippen Method
mcvol	211.000	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
tb	643.49	K	Cheméo Relay (1.0)
tc	854.53	K	Cheméo Relay (1.0)
tf	319.08	K	Cheméo Relay (1.0)

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:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59950117&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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