benzyl phenyl sulfoxide

Inchi: InChI=1S/C13H12OS/c14-15(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10H,11H2
InchiKey: FBPGAWABXWMRAR-UHFFFAOYSA-N
Formula: C13H12OS
SMILES: O=S(Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 216.31

Physical Properties

Property code	Value	Unit	Source
hf	102.75	kJ/mol	Cheméo Relay (1.0)
hfus	25.26	kJ/mol	Joback Method
hvap	99.36	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
logp	2.994		Crippen Method
mcvol	168.730	ml/mol	McGowan Method
tb	623.07	K	Cheméo Relay (1.0)
tf	393.00 ± 3.00	K	NIST Webbook
tf	396.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.01	J/mol×K	608.48	Joback Method
cpg	409.58	J/mol×K	649.90	Joback Method
cpg	424.78	J/mol×K	691.32	Joback Method
cpg	438.66	J/mol×K	732.74	Joback Method
cpg	451.29	J/mol×K	774.16	Joback Method
cpg	462.72	J/mol×K	815.58	Joback Method
cpg	473.04	J/mol×K	857.00	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C833829&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point