

Benzyl phenyl sulfide

Other names:	1,2-Diphenyl-1-thiaethane Benzyl phenyl sulfide Phenyl benzyl sulfide Sulfide, benzyl phenyl benzyl phenyl sulphide
Inchi:	InChI=1S/C13H12S/c1-3-7-12(8-4-1)11-14-13-9-5-2-6-10-13/h1-10H,11H2
InchiKey:	LKMCJXXOBRCATQ-UHFFFAOYSA-N
Formula:	C13H12S
SMILES:	c1ccc(CSc2ccccc2)cc1
Mol. weight [g/mol]:	200.31

Physical Properties

Property code	Value	Unit	Source
af	0.3738		Cheméo Relay (1.0)
gf	316.52	kJ/mol	Joback Method
hf	225.59	kJ/mol	Cheméo Relay (1.0)
hfus	21.64	kJ/mol	Joback Method
hsub	98.40 ± 1.40	kJ/mol	NIST Webbook
hvap	79.79	kJ/mol	Cheméo Relay (1.0)
ie	7.87 ± 0.02	eV	NIST Webbook
log10ws	-4.72		Cheméo Relay (1.0)
logp	3.979		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	577.46	K	Cheméo Relay (1.0)
tc	819.41	K	Cheméo Relay (1.0)
tf	324.59	K	Cheméo Relay (1.0)
vc	0.596	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.75	J/mol×K	618.98	Joback Method
cpg	394.36	J/mol×K	663.10	Joback Method

cpg	409.52	J/mol×K	707.21	Joback Method
cpg	423.31	J/mol×K	751.33	Joback Method
cpg	435.82	J/mol×K	795.45	Joback Method
cpg	447.13	J/mol×K	839.56	Joback Method
cpg	457.34	J/mol×K	883.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	470.20	K	3.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C831914&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
hsub:	Enthalpy of sublimation 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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