2-(Methylthio)benzoic acid, 3-iodobenzyl ester

Inchi: InChI=1S/C15H13IO2S/c1-19-14-8-3-2-7-13(14)15(17)18-10-11-5-4-6-12(16)9-11/h2-9H
InchiKey: YPNHDJSSNSEBNA-UHFFFAOYSA-N
Formula: C15H13IO2S
SMILES: CSc1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 384.23

Physical Properties

Property code	Value	Unit	Source
gf	138.30	kJ/mol	Joback Method
hf	-28.87	kJ/mol	Joback Method
hfus	33.23	kJ/mol	Joback Method
hvap	80.21	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.370		Crippen Method
mcvol	224.300	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	2660.00		NIST Webbook
tb	844.13	K	Joback Method
tc	1121.48	K	Joback Method
tf	501.31	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.85	J/mol×K	844.13	Joback Method
cpg	569.96	J/mol×K	890.35	Joback Method
cpg	580.70	J/mol×K	936.58	Joback Method
cpg	590.14	J/mol×K	982.80	Joback Method
cpg	598.36	J/mol×K	1029.03	Joback Method
cpg	605.42	J/mol×K	1075.25	Joback Method
cpg	611.40	J/mol×K	1121.48	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=U375052&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume