4-(Methylthio)benzoic acid, 3-bromobenzyl ester

Inchi: InChI=1S/C15H13BrO2S/c1-19-14-7-5-12(6-8-14)15(17)18-10-11-3-2-4-13(16)9-11/h2-9
InchiKey: FLQQLMSMHSJCAK-UHFFFAOYSA-N
Formula: C15H13BrO2S
SMILES: CSc1ccc(C(=O)OCc2cccc(Br)c2)cc1
Mol. weight [g/mol]: 337.23

Physical Properties

Property code	Value	Unit	Source
gf	94.50	kJ/mol	Joback Method
hf	-79.41	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	77.27	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.528		Crippen Method
mcvol	215.980	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	2627.00		NIST Webbook
rinpol	2627.00		NIST Webbook
tb	817.15	K	Joback Method
tc	1080.96	K	Joback Method
tf	503.05	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.48	J/mol×K	817.15	Joback Method
cpg	561.98	J/mol×K	861.12	Joback Method
cpg	573.19	J/mol×K	905.09	Joback Method
cpg	583.16	J/mol×K	949.06	Joback Method
cpg	591.95	J/mol×K	993.03	Joback Method
cpg	599.62	J/mol×K	1037.00	Joback Method
cpg	606.21	J/mol×K	1080.96	Joback Method

Sources

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=U375062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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