2-(Methylthio)benzoic acid, 4-bromophenethyl ester

Inchi: InChI=1S/C16H15BrO2S/c1-20-15-5-3-2-4-14(15)16(18)19-11-10-12-6-8-13(17)9-7-12/h

InchiKey: NYKVGYIBLDHIQJ-UHFFFAOYSA-N

Formula: C16H15BrO2S

SMILES: CSc1ccccc1C(=O)OCCc1ccc(Br)cc1

Mol. weight [g/mol]: 351.26

Physical Properties

Property code	Value	Unit	Source
gf	102.92	kJ/mol	Joback Method
hf	-100.05	kJ/mol	Joback Method
hfus	36.70	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.571		Crippen Method
mcvol	230.070	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	2649.00		NIST Webbook
tb	840.03	K	Joback Method
tc	1098.20	K	Joback Method
tf	514.32	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.71	J/mol×K	840.03	Joback Method
cpg	616.49	J/mol×K	883.06	Joback Method
cpg	627.97	J/mol×K	926.09	Joback Method
cpg	638.21	J/mol×K	969.12	Joback Method
cpg	647.27	J/mol×K	1012.15	Joback Method
cpg	655.21	J/mol×K	1055.17	Joback Method
cpg	662.09	J/mol×K	1098.20	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=U375049&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