3-Methoxybenzoic acid, 3-bromobenzyl ester

Inchi: InChI=1S/C15H13BrO3/c1-18-14-7-3-5-12(9-14)15(17)19-10-11-4-2-6-13(16)8-11/h2-9H
InchiKey: IWJSJNNRJBUJAB-UHFFFAOYSA-N
Formula: C15H13BrO3
SMILES: COc1cccc(C(=O)OCc2cccc(Br)c2)c1
Mol. weight [g/mol]: 321.17

Physical Properties

Property code	Value	Unit	Source
gf	-43.62	kJ/mol	Joback Method
hf	-253.50	kJ/mol	Joback Method
hfus	31.17	kJ/mol	Joback Method
hvap	72.86	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.815		Crippen Method
mcvol	205.500	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	2343.00		NIST Webbook
tb	770.79	K	Joback Method
tc	1016.42	K	Joback Method
tf	490.88	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.95	J/mol×K	770.79	Joback Method
cpg	580.43	J/mol×K	975.48	Joback Method
cpg	571.72	J/mol×K	934.54	Joback Method
cpg	561.95	J/mol×K	893.60	Joback Method
cpg	551.09	J/mol×K	852.67	Joback Method
cpg	539.10	J/mol×K	811.73	Joback Method
cpg	588.11	J/mol×K	1016.42	Joback Method
dvisc	0.0000931	Pa×s	770.79	Joback Method
dvisc	0.0001144	Pa×s	724.14	Joback Method

dvisc	0.0001446	Pa×s	677.49	Joback Method
dvisc	0.0001892	Pa×s	630.84	Joback Method
dvisc	0.0002584	Pa×s	584.18	Joback Method
dvisc	0.0003725	Pa×s	537.53	Joback Method
dvisc	0.0005757	Pa×s	490.88	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=U374927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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