

4-Methoxybenzoic acid, 3-bromobenzyl ester

Inchi:	InChI=1S/C15H13BrO3/c1-18-14-7-5-12(6-8-14)15(17)19-10-11-3-2-4-13(16)9-11/h2-9H
InchiKey:	NFHOQWKGIXYHQM-UHFFFAOYSA-N
Formula:	C15H13BrO3
SMILES:	COc1ccc(C(=O)OCc2cccc(Br)c2)cc1
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	2409.00		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/molxK	770.79	Joback Method
cpg	539.10	J/molxK	811.73	Joback Method
cpg	551.09	J/molxK	852.67	Joback Method
cpg	561.95	J/molxK	893.60	Joback Method
cpg	571.72	J/molxK	934.54	Joback Method
cpg	580.43	J/molxK	975.48	Joback Method
cpg	588.11	J/molxK	1016.42	Joback Method
dvisc	0.0005757	Paxs	490.88	Joback Method
dvisc	0.0003725	Paxs	537.53	Joback Method

dvisc	0.0002584	Paxs	584.18	Joback Method
dvisc	0.0001892	Paxs	630.84	Joback Method
dvisc	0.0001446	Paxs	677.49	Joback Method
dvisc	0.0001144	Paxs	724.14	Joback Method
dvisc	0.0000931	Paxs	770.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U374936&Units=SI

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

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