3-Methoxy-4-benzyloxyphenylacetic acid, methyl ester

Inchi: InChI=1S/C17H18O4/c1-19-16-10-14(11-17(18)20-2)8-9-15(16)21-12-13-6-4-3-5-7-13/h3

InchiKey: LRUAKAWBLZSQMZ-UHFFFAOYSA-N

Formula: C17H18O4

SMILES: COC(=O)Cc1ccc(OCc2ccccc2)c(OC)c1

Mol. weight [g/mol]: 286.32

Physical Properties

Property code	Value	Unit	Source
gf	-146.10	kJ/mol	Joback Method
hf	-453.33	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	73.29	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.990		Crippen Method
mcvol	222.050	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	2185.30		NIST Webbook
rinpol	2145.40		NIST Webbook
tb	772.81	K	Joback Method
tc	997.61	K	Joback Method
tf	475.85	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.51	J/mol×K	772.81	Joback Method
cpg	639.64	J/mol×K	810.28	Joback Method
cpg	653.56	J/mol×K	847.74	Joback Method
cpg	666.27	J/mol×K	885.21	Joback Method
cpg	677.78	J/mol×K	922.68	Joback Method
cpg	688.09	J/mol×K	960.15	Joback Method
cpg	697.22	J/mol×K	997.61	Joback Method
dvisc	0.0004864	Pa×s	475.85	Joback Method

dvisc	0.0002972	Pa×s	525.34	Joback Method
dvisc	0.0001977	Pa×s	574.84	Joback Method
dvisc	0.0001403	Pa×s	624.33	Joback Method
dvisc	0.0001047	Pa×s	673.82	Joback Method
dvisc	0.0000813	Pa×s	723.32	Joback Method
dvisc	0.0000652	Pa×s	772.81	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=R157825&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