2-Methoxybenzoic acid, 2-methoxybenzyl ester

Inchi: InChI=1S/C16H16O4/c1-18-14-9-5-3-7-12(14)11-20-16(17)13-8-4-6-10-15(13)19-2/h3-10

InchiKey: NNLUYJMVNPPSPE-UHFFFAOYSA-N

Formula: C16H16O4

SMILES: COc1ccccc1COC(=O)c1ccccc1OC

Mol. weight [g/mol]: 272.30

Physical Properties

Property code	Value	Unit	Source
gf	-154.52	kJ/mol	Joback Method
hf	-432.69	kJ/mol	Joback Method
hfus	29.66	kJ/mol	Joback Method
hvap	71.06	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.061		Crippen Method
mcvol	207.960	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	2234.00		NIST Webbook
tb	749.93	K	Joback Method
tc	978.33	K	Joback Method
tf	464.58	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.92	J/mol×K	749.93	Joback Method
cpg	584.80	J/mol×K	788.00	Joback Method
cpg	598.50	J/mol×K	826.06	Joback Method
cpg	611.02	J/mol×K	864.13	Joback Method
cpg	622.38	J/mol×K	902.20	Joback Method
cpg	632.55	J/mol×K	940.26	Joback Method
cpg	641.56	J/mol×K	978.33	Joback Method
dvisc	0.0005232	Pa×s	464.58	Joback Method
dvisc	0.0003242	Pa×s	512.14	Joback Method

dvisc	0.0002180	Pa×s	559.70	Joback Method
dvisc	0.0001559	Pa×s	607.25	Joback Method
dvisc	0.0001171	Pa×s	654.81	Joback Method
dvisc	0.0000914	Pa×s	702.37	Joback Method
dvisc	0.0000737	Pa×s	749.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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