Benzoic acid, 3-methoxy-, 4-benzyloxyphenyl ester

Other names: m-Anisic acid, 4-benzyloxyphenyl ester
Inchi: InChI=1S/C21H18O4/c1-23-20-9-5-8-17(14-20)21(22)25-19-12-10-18(11-13-19)24-15-16
InchiKey: PCDDKDJQBZUEQW-UHFFFAOYSA-N
Formula: C21H18O4
SMILES: COc1cccc(C(=O)Oc2ccc(OCc3ccccc3)cc2)c1
Mol. weight [g/mol]: 334.37
CAS: 306743-72-6

Physical Properties

Property code	Value	Unit	Source
gf	-0.01	kJ/mol	Joback Method
hf	-299.36	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	84.47	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.493		Crippen Method
mcvol	254.650	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	2907.00		NIST Webbook
rinpol	2907.00		NIST Webbook
tb	891.01	K	Joback Method
tc	1137.48	K	Joback Method
tf	547.35	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.04	J/mol×K	891.01	Joback Method
cpg	766.61	J/mol×K	932.09	Joback Method
cpg	778.61	J/mol×K	973.17	Joback Method
cpg	789.05	J/mol×K	1014.25	Joback Method
cpg	797.99	J/mol×K	1055.33	Joback Method
cpg	805.46	J/mol×K	1096.40	Joback Method

cpg	811.50	J/mol×K	1137.48	Joback Method
dvisc	0.0003075	Pa×s	547.35	Joback Method
dvisc	0.0001862	Pa×s	604.63	Joback Method
dvisc	0.0001230	Pa×s	661.90	Joback Method
dvisc	0.0000868	Pa×s	719.18	Joback Method
dvisc	0.0000645	Pa×s	776.46	Joback Method
dvisc	0.0000499	Pa×s	833.73	Joback Method
dvisc	0.0000399	Pa×s	891.01	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C306743726&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

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.