3-Benzyloxy-4-methoxybenzoic acid

Other names: Benzoic acid, 4-methoxy-3-(phenylmethoxy)-
Benzoic acid, 3-benzyloxy-4-methoxy-
3-benzyloxy-p-anisic acid
Inchi: InChI=1S/C15H14O4/c1-18-13-8-7-12(15(16)17)9-14(13)19-10-11-5-3-2-4-6-11/h2-9H,10
InchiKey: YPDXIGBSOBESNI-UHFFFAOYSA-N
Formula: C15H14O4
SMILES: COc1ccc(C(=O)O)cc1OCc1ccccc1
Mol. weight [g/mol]: 258.27
CAS: 58452-00-9

Physical Properties

Property code	Value	Unit	Source
gf	-194.76	kJ/mol	Joback Method
hf	-432.06	kJ/mol	Joback Method
hfus	29.97	kJ/mol	Joback Method
hvap	83.11	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.972		Crippen Method
mcvol	193.870	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
tb	796.81	K	Joback Method
tc	1016.28	K	Joback Method
tf	491.90	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.94	J/mol×K	796.81	Joback Method
cpg	553.60	J/mol×K	833.39	Joback Method
cpg	564.29	J/mol×K	869.97	Joback Method
cpg	574.04	J/mol×K	906.55	Joback Method
cpg	582.85	J/mol×K	943.12	Joback Method
cpg	590.75	J/mol×K	979.70	Joback Method

cpg	597.76	J/mol×K	1016.28	Joback Method
dvisc	0.0004137	Pa×s	491.90	Joback Method
dvisc	0.0001970	Pa×s	542.72	Joback Method
dvisc	0.0001065	Pa×s	593.54	Joback Method
dvisc	0.0000635	Pa×s	644.36	Joback Method
dvisc	0.0000408	Pa×s	695.17	Joback Method
dvisc	0.0000278	Pa×s	745.99	Joback Method
dvisc	0.0000200	Pa×s	796.81	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58452009&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume