Propanoic acid, 3-(4-benzyloxyphenyl)-, methyl ester

Other names: Methyl 3-[4-(benzyloxy)phenyl]propanoate
3-(4-Benzyloxyphenyl)-propionic acid, methyl ester

Inchi: InChI=1S/C17H18O3/c1-19-17(18)12-9-14-7-10-16(11-8-14)20-13-15-5-3-2-4-6-15/h2-8,

InchiKey: XAAMAAXKDLWBKO-UHFFFAOYSA-N

Formula: C17H18O3

SMILES: COC(=O)CCc1ccc(OCc2ccccc2)cc1

Mol. weight [g/mol]: 270.32

CAS: 24807-40-7

Physical Properties

Property code	Value	Unit	Source
gf	-31.47	kJ/mol	Joback Method
hf	-309.64	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.371		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	2178.00		NIST Webbook
rinpol	2178.00		NIST Webbook
tb	745.41	K	Joback Method
tc	971.98	K	Joback Method
tf	441.10	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.41	J/mol×K	745.41	Joback Method
cpg	614.18	J/mol×K	783.17	Joback Method
cpg	628.74	J/mol×K	820.93	Joback Method
cpg	642.13	J/mol×K	858.69	Joback Method
cpg	654.37	J/mol×K	896.46	Joback Method

cpg	665.49	J/mol×K	934.22	Joback Method
cpg	675.53	J/mol×K	971.98	Joback Method
dvisc	0.0007907	Pa×s	441.10	Joback Method
dvisc	0.0004493	Pa×s	491.82	Joback Method
dvisc	0.0002838	Pa×s	542.54	Joback Method
dvisc	0.0001939	Pa×s	593.25	Joback Method
dvisc	0.0001407	Pa×s	643.97	Joback Method
dvisc	0.0001070	Pa×s	694.69	Joback Method
dvisc	0.0000844	Pa×s	745.41	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=C24807407&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