Benzoic acid, 2-methyl-, 4-benzyloxyphenyl ester

Other names: o-Toluylic acid, 4-benzyloxyphenyl ester
Inchi: InChI=1S/C21H18O3/c1-16-7-5-6-10-20(16)21(22)24-19-13-11-18(12-14-19)23-15-17-8-
InchiKey: VAUDJIBDOMUTDP-UHFFFAOYSA-N
Formula: C21H18O3
SMILES: Cc1ccccc1C(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 318.37
CAS: 306743-69-1

Physical Properties

Property code	Value	Unit	Source
gf	104.99	kJ/mol	Joback Method
hf	-167.14	kJ/mol	Joback Method
hfus	35.47	kJ/mol	Joback Method
hvap	82.06	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	4.793		Crippen Method
mcvol	248.780	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	2701.00		NIST Webbook
rinpol	2701.00		NIST Webbook
tb	868.59	K	Joback Method
tc	1118.04	K	Joback Method
tf	525.12	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.51	J/mol×K	868.59	Joback Method
cpg	784.28	J/mol×K	1076.47	Joback Method
cpg	775.49	J/mol×K	1034.89	Joback Method
cpg	765.38	J/mol×K	993.32	Joback Method
cpg	753.89	J/mol×K	951.74	Joback Method
cpg	740.96	J/mol×K	910.17	Joback Method

cpg	791.81	J/mol×K	1118.04	Joback Method
dvisc	0.0000528	Pa×s	868.59	Joback Method
dvisc	0.0000662	Pa×s	811.34	Joback Method
dvisc	0.0000858	Pa×s	754.10	Joback Method
dvisc	0.0001161	Pa×s	696.86	Joback Method
dvisc	0.0001658	Pa×s	639.61	Joback Method
dvisc	0.0002540	Pa×s	582.37	Joback Method
dvisc	0.0004271	Pa×s	525.12	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=C306743691&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

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