p-Toluic acid, 4-benzyloxyphenyl ester

Other names: p-Toluylic acid, 4-benzyloxyphenyl ester
Inchi: InChI=1S/C21H18O3/c1-16-7-9-18(10-8-16)21(22)24-20-13-11-19(12-14-20)23-15-17-5-
InchiKey: UEXNAAFGIOCCME-UHFFFAOYSA-N
Formula: C21H18O3
SMILES: Cc1ccc(C(=O)Oc2ccc(OCc3ccccc3)cc2)cc1
Mol. weight [g/mol]: 318.37

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	2784.00		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

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=U307772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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