4-Butylbenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C24H24O3/c1-2-3-7-19-10-12-21(13-11-19)24(25)27-23-16-14-22(15-17-23)26
InchiKey: XGUHUAHNDPETLF-UHFFFAOYSA-N
Formula: C24H24O3
SMILES: CCCCc1ccc(C(=O)Oc2ccc(OCc3ccccc3)cc2)cc1
Mol. weight [g/mol]: 360.45

Physical Properties

Property code	Value	Unit	Source
gf	130.25	kJ/mol	Joback Method
hf	-229.06	kJ/mol	Joback Method
hfus	43.24	kJ/mol	Joback Method
hvap	88.74	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	5.827		Crippen Method
mcvol	291.050	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	3197.00		NIST Webbook
tb	937.23	K	Joback Method
tc	1176.94	K	Joback Method
tf	558.93	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.97	J/mol×K	937.23	Joback Method
cpg	914.34	J/mol×K	977.18	Joback Method
cpg	927.22	J/mol×K	1017.13	Joback Method
cpg	938.69	J/mol×K	1057.08	Joback Method
cpg	948.81	J/mol×K	1097.04	Joback Method
cpg	957.65	J/mol×K	1136.99	Joback Method
cpg	965.29	J/mol×K	1176.94	Joback Method
dvisc	0.0003205	Pa×s	558.93	Joback Method
dvisc	0.0001840	Pa×s	621.98	Joback Method

dvisc	0.0001170	Pa×s	685.03	Joback Method
dvisc	0.0000803	Pa×s	748.08	Joback Method
dvisc	0.0000585	Pa×s	811.13	Joback Method
dvisc	0.0000445	Pa×s	874.18	Joback Method
dvisc	0.0000352	Pa×s	937.23	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307511&Units=SI

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