4-Ethylbenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C22H20O3/c1-2-17-8-10-19(11-9-17)22(23)25-21-14-12-20(13-15-21)24-16-18
InchiKey: YGLUCBMXAHYNRN-UHFFFAOYSA-N
Formula: C22H20O3
SMILES: CCc1ccc(C(=O)Oc2ccc(OCc3ccccc3)cc2)cc1
Mol. weight [g/mol]: 332.39

Physical Properties

Property code	Value	Unit	Source
gf	113.41	kJ/mol	Joback Method
hf	-187.78	kJ/mol	Joback Method
hfus	38.06	kJ/mol	Joback Method
hvap	84.28	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.047		Crippen Method
mcvol	262.870	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	2892.00		NIST Webbook
tb	891.47	K	Joback Method
tc	1136.96	K	Joback Method
tf	536.39	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.63	J/mol×K	891.47	Joback Method
cpg	841.51	J/mol×K	1096.05	Joback Method
cpg	832.67	J/mol×K	1055.13	Joback Method
cpg	822.53	J/mol×K	1014.22	Joback Method
cpg	811.02	J/mol×K	973.30	Joback Method
cpg	798.08	J/mol×K	932.39	Joback Method
cpg	849.11	J/mol×K	1136.96	Joback Method
dvisc	0.0000463	Pa×s	891.47	Joback Method
dvisc	0.0000582	Pa×s	832.29	Joback Method

dvisc	0.0000757	Pa×s	773.11	Joback Method
dvisc	0.0001030	Pa×s	713.93	Joback Method
dvisc	0.0001482	Pa×s	654.75	Joback Method
dvisc	0.0002290	Pa×s	595.57	Joback Method
dvisc	0.0003898	Pa×s	536.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307129&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume