O-anisic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C21H18O4/c1-23-20-10-6-5-9-19(20)21(22)25-18-13-11-17(12-14-18)24-15-16
InchiKey: VFZAOEBIFQDMTQ-UHFFFAOYSA-N
Formula: C21H18O4
SMILES: COc1ccccc1C(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 334.37

Physical Properties

Property code	Value	Unit	Source
hf	-330.15	kJ/mol	Cheméo Relay (1.0)
hfus	36.65	kJ/mol	Joback Method
hvap	113.78	kJ/mol	Cheméo Relay (1.0)
ie	7.88	eV	Cheméo Relay (1.0)
log10ws	-5.38		Cheméo Relay (1.0)
logp	4.493		Crippen Method
mcvol	254.650	ml/mol	McGowan Method
rinpol	2863.00		NIST Webbook
rinpol	2863.00		NIST Webbook
tb	698.69	K	Cheméo Relay (1.0)
tf	364.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.04	J/mol×K	891.01	Joback Method
cpg	766.61	J/mol×K	932.09	Joback Method
cpg	778.61	J/mol×K	973.17	Joback Method
cpg	789.05	J/mol×K	1014.25	Joback Method
cpg	797.99	J/mol×K	1055.33	Joback Method
cpg	805.46	J/mol×K	1096.40	Joback Method
cpg	811.50	J/mol×K	1137.48	Joback Method
dvisc	0.0003075	Pa×s	547.35	Joback Method
dvisc	0.0001862	Pa×s	604.63	Joback Method
dvisc	0.0001230	Pa×s	661.90	Joback Method
dvisc	0.0000868	Pa×s	719.18	Joback Method

dvisc	0.0000645	Pa×s	776.46	Joback Method
dvisc	0.0000499	Pa×s	833.73	Joback Method
dvisc	0.0000399	Pa×s	891.01	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307797&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point