3-Phenylpropionic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C22H20O3/c23-22(16-11-18-7-3-1-4-8-18)25-21-14-12-20(13-15-21)24-17-19-

InchiKey: ROBBAEHOOIWETD-UHFFFAOYSA-N

Formula: C22H20O3

SMILES: O=C(CCc1ccccc1)Oc1ccc(OCc2ccccc2)cc1

Mol. weight [g/mol]: 332.39

Physical Properties

Property code	Value	Unit	Source
gf	123.04	kJ/mol	Joback Method
hf	-176.31	kJ/mol	Joback Method
hfus	38.45	kJ/mol	Joback Method
hvap	83.62	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.804		Crippen Method
mcvol	262.870	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	886.49	K	Joback Method
tc	1131.29	K	Joback Method
tf	523.87	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.86	J/mol×K	886.49	Joback Method
cpg	799.42	J/mol×K	927.29	Joback Method
cpg	812.50	J/mol×K	968.09	Joback Method
cpg	824.16	J/mol×K	1008.89	Joback Method
cpg	834.47	J/mol×K	1049.69	Joback Method
cpg	843.52	J/mol×K	1090.49	Joback Method
cpg	851.37	J/mol×K	1131.29	Joback Method
dvisc	0.0004446	Pa×s	523.87	Joback Method

dvisc	0.0002498	Pa×s	584.31	Joback Method
dvisc	0.0001563	Pa×s	644.74	Joback Method
dvisc	0.0001060	Pa×s	705.18	Joback Method
dvisc	0.0000764	Pa×s	765.62	Joback Method
dvisc	0.0000578	Pa×s	826.05	Joback Method
dvisc	0.0000454	Pa×s	886.49	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=U307788&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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