Phenylacetic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C21H18O3/c22-21(15-17-7-3-1-4-8-17)24-20-13-11-19(12-14-20)23-16-18-9-5
InchiKey: OYNXINLGCAVEFI-UHFFFAOYSA-N
Formula: C21H18O3
SMILES: O=C(Cc1ccccc1)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 318.37

Physical Properties

Property code	Value	Unit	Source
gf	114.62	kJ/mol	Joback Method
hf	-155.67	kJ/mol	Joback Method
hfus	35.85	kJ/mol	Joback Method
hvap	81.40	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.414		Crippen Method
mcvol	248.780	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	2680.00		NIST Webbook
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tb	863.61	K	Joback Method
tc	1112.38	K	Joback Method
tf	512.60	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.78	J/mol×K	863.61	Joback Method
cpg	742.35	J/mol×K	905.07	Joback Method
cpg	755.41	J/mol×K	946.53	Joback Method
cpg	767.03	J/mol×K	987.99	Joback Method
cpg	777.30	J/mol×K	1029.45	Joback Method
cpg	786.28	J/mol×K	1070.92	Joback Method
cpg	794.04	J/mol×K	1112.38	Joback Method
dvisc	0.0004889	Pa×s	512.60	Joback Method

dvisc	0.0002779	Pa×s	571.10	Joback Method
dvisc	0.0001754	Pa×s	629.60	Joback Method
dvisc	0.0001197	Pa×s	688.11	Joback Method
dvisc	0.0000868	Pa×s	746.61	Joback Method
dvisc	0.0000659	Pa×s	805.11	Joback Method
dvisc	0.0000520	Pa×s	863.61	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=U307538&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