2,2-Dimethylpropanoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C18H20O3/c1-18(2,3)17(19)21-16-11-9-15(10-12-16)20-13-14-7-5-4-6-8-14/h4

InchiKey: YOCHWZIIVKJIAX-UHFFFAOYSA-N

Formula: C18H20O3

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

Mol. weight [g/mol]: 284.35

Physical Properties

Property code	Value	Unit	Source
gf	-20.21	kJ/mol	Joback Method
hf	-339.03	kJ/mol	Joback Method
hfus	26.63	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.217		Crippen Method
mcvol	230.270	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
tb	765.06	K	Joback Method
tc	999.30	K	Joback Method
tf	454.79	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.47	J/mol×K	765.06	Joback Method
cpg	671.91	J/mol×K	804.10	Joback Method
cpg	687.00	J/mol×K	843.14	Joback Method
cpg	700.81	J/mol×K	882.18	Joback Method
cpg	713.40	J/mol×K	921.22	Joback Method
cpg	724.83	J/mol×K	960.26	Joback Method
cpg	735.19	J/mol×K	999.30	Joback Method
dvisc	0.0007073	Pa×s	454.79	Joback Method

dvisc	0.0003813	Pa×s	506.50	Joback Method
dvisc	0.0002305	Pa×s	558.21	Joback Method
dvisc	0.0001518	Pa×s	609.92	Joback Method
dvisc	0.0001067	Pa×s	661.64	Joback Method
dvisc	0.0000789	Pa×s	713.35	Joback Method
dvisc	0.0000608	Pa×s	765.06	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=U308047&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