Cyclopropanecarboxylic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C17H16O3/c18-17(14-6-7-14)20-16-10-8-15(9-11-16)19-12-13-4-2-1-3-5-13/h1

InchiKey: HGGWJLDXGZHPDB-UHFFFAOYSA-N

Formula: C17H16O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C1CC1

Mol. weight [g/mol]: 268.31

Physical Properties

Property code	Value	Unit	Source
gf	29.28	kJ/mol	Joback Method
hf	-236.84	kJ/mol	Joback Method
hfus	29.59	kJ/mol	Joback Method
hvap	70.13	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.581		Crippen Method
mcvol	205.320	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	752.15	K	Joback Method
tc	992.66	K	Joback Method
tf	459.04	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.24	J/mol×K	752.15	Joback Method
cpg	598.25	J/mol×K	792.24	Joback Method
cpg	612.95	J/mol×K	832.32	Joback Method
cpg	626.43	J/mol×K	872.41	Joback Method
cpg	638.76	J/mol×K	912.49	Joback Method
cpg	650.01	J/mol×K	952.58	Joback Method
cpg	660.27	J/mol×K	992.66	Joback Method
dvisc	0.0012114	Pa×s	459.04	Joback Method

dvisc	0.0008133	Pa×s	507.89	Joback Method
dvisc	0.0005856	Pa×s	556.74	Joback Method
dvisc	0.0004446	Pa×s	605.60	Joback Method
dvisc	0.0003517	Pa×s	654.45	Joback Method
dvisc	0.0002874	Pa×s	703.30	Joback Method
dvisc	0.0002412	Pa×s	752.15	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=U307529&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