Carbonic acid, isobutyl 4-benzyloxyphenyl ester

Inchi: InChI=1S/C18H20O4/c1-14(2)12-21-18(19)22-17-10-8-16(9-11-17)20-13-15-6-4-3-5-7-15

InchiKey: DWPQVUKZZZKNOC-UHFFFAOYSA-N

Formula: C18H20O4

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

Mol. weight [g/mol]: 300.35

Physical Properties

Property code	Value	Unit	Source
gf	-130.49	kJ/mol	Joback Method
hf	-467.78	kJ/mol	Joback Method
hfus	31.71	kJ/mol	Joback Method
hvap	74.46	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.437		Crippen Method
mcvol	236.140	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
tb	790.27	K	Joback Method
tc	1014.75	K	Joback Method
tf	459.60	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.66	J/mol×K	790.27	Joback Method
cpg	697.33	J/mol×K	827.68	Joback Method
cpg	711.69	J/mol×K	865.10	Joback Method
cpg	724.77	J/mol×K	902.51	Joback Method
cpg	736.58	J/mol×K	939.92	Joback Method
cpg	747.14	J/mol×K	977.34	Joback Method
cpg	756.46	J/mol×K	1014.75	Joback Method
dvisc	0.0005967	Pa×s	459.60	Joback Method

dvisc	0.0003203	Pa×s	514.71	Joback Method
dvisc	0.0001939	Pa×s	569.82	Joback Method
dvisc	0.0001282	Pa×s	624.93	Joback Method
dvisc	0.0000907	Pa×s	680.05	Joback Method
dvisc	0.0000676	Pa×s	735.16	Joback Method
dvisc	0.0000524	Pa×s	790.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357839&Units=SI
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

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