Carbonic acid, propargyl 4-benzyloxyphenyl ester

Inchi: InChI=1S/C17H14O4/c1-2-12-19-17(18)21-16-10-8-15(9-11-16)20-13-14-6-4-3-5-7-14/h1

InchiKey: GSOABTQNZZAHGE-UHFFFAOYSA-N

Formula: C17H14O4

SMILES: C#CCOC(=O)Oc1ccc(OCc2ccccc2)cc1

Mol. weight [g/mol]: 282.29

Physical Properties

Property code	Value	Unit	Source
gf	86.60	kJ/mol	Joback Method
hf	-149.96	kJ/mol	Joback Method
hfus	35.62	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.414		Crippen Method
mcvol	213.450	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	2335.00		NIST Webbook
tb	757.95	K	Joback Method
tc	995.17	K	Joback Method
tf	510.30	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.23	J/mol×K	757.95	Joback Method
cpg	588.54	J/mol×K	797.49	Joback Method
cpg	601.62	J/mol×K	837.02	Joback Method
cpg	613.50	J/mol×K	876.56	Joback Method
cpg	624.21	J/mol×K	916.10	Joback Method
cpg	633.76	J/mol×K	955.63	Joback Method
cpg	642.17	J/mol×K	995.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357911&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
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