

Carbonic acid, 2-methoxyethyl 4-benzyloxyphenyl ester

Inchi:	InChI=1S/C17H18O5/c1-19-11-12-20-17(18)22-16-9-7-15(8-10-16)21-13-14-5-3-2-4-6-14
InchiKey:	IHGDDUZRHUFVPA-UHFFFAOYSA-N
Formula:	C17H18O5
SMILES:	COCCOC(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	302.32

Physical Properties

Property code	Value	Unit	Source
gf	-241.47	kJ/mol	Joback Method
hf	-574.08	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.427		Crippen Method
mcvol	227.920	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinsol	2443.00		NIST Webbook
tb	790.25	K	Joback Method
tc	1012.13	K	Joback Method
tf	485.56	K	Joback Method
vc	0.850	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.67	J/molxK	790.25	Joback Method
cpg	667.37	J/molxK	827.23	Joback Method
cpg	680.81	J/molxK	864.21	Joback Method
cpg	692.99	J/molxK	901.19	Joback Method
cpg	703.90	J/molxK	938.17	Joback Method
cpg	713.54	J/molxK	975.15	Joback Method
cpg	721.91	J/molxK	1012.13	Joback Method
dvisc	0.0004091	Paxs	485.56	Joback Method
dvisc	0.0002435	Paxs	536.34	Joback Method

dvisc	0.0001585	Paxs	587.12	Joback Method
dvisc	0.0001105	Paxs	637.90	Joback Method
dvisc	0.0000812	Paxs	688.69	Joback Method
dvisc	0.0000623	Paxs	739.47	Joback Method
dvisc	0.0000494	Paxs	790.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U357876&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

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