Carbonic acid, isobutyl 4-methoxyphenyl ester

Inchi: InChI=1S/C12H16O4/c1-9(2)8-15-12(13)16-11-6-4-10(14-3)5-7-11/h4-7,9H,8H2,1-3H3
InchiKey: DVHVQXDNFHZQJY-UHFFFAOYSA-N
Formula: C12H16O4
SMILES: COc1ccc(OC(=O)OCC(C)C)cc1
Mol. weight [g/mol]: 224.25

Physical Properties

Property code	Value	Unit	Source
gf	-293.42	kJ/mol	Joback Method
hf	-580.47	kJ/mol	Joback Method
hfus	22.13	kJ/mol	Joback Method
hvap	58.83	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.867		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	1661.00		NIST Webbook
rinpol	1661.00		NIST Webbook
tb	626.31	K	Joback Method
tc	833.16	K	Joback Method
tf	365.56	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.46	J/mol×K	626.31	Joback Method
cpg	511.18	J/mol×K	798.68	Joback Method
cpg	499.64	J/mol×K	764.21	Joback Method
cpg	487.28	J/mol×K	729.73	Joback Method
cpg	474.13	J/mol×K	695.26	Joback Method
cpg	460.19	J/mol×K	660.78	Joback Method
cpg	521.91	J/mol×K	833.16	Joback Method
dvisc	0.0001072	Pa×s	626.31	Joback Method

dvisc	0.0001372	Pa×s	582.85	Joback Method
dvisc	0.0001828	Pa×s	539.39	Joback Method
dvisc	0.0002559	Pa×s	495.93	Joback Method
dvisc	0.0003823	Pa×s	452.48	Joback Method
dvisc	0.0006221	Pa×s	409.02	Joback Method
dvisc	0.0011363	Pa×s	365.56	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=U357834&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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