

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
mvol	175.360	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	1661.00		NIST Webbook
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tb	626.31	K	Joback Method
tc	833.16	K	Joback Method
tf	365.56	K	Joback Method
vc	0.653	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.46	J/molxK	626.31	Joback Method
cpg	460.19	J/molxK	660.78	Joback Method
cpg	474.13	J/molxK	695.26	Joback Method
cpg	487.28	J/molxK	729.73	Joback Method
cpg	499.64	J/molxK	764.21	Joback Method
cpg	511.18	J/molxK	798.68	Joback Method
cpg	521.91	J/molxK	833.16	Joback Method
dvisc	0.0011363	Paxs	365.56	Joback Method

dvisc	0.0006221	Paxs	409.02	Joback Method
dvisc	0.0003823	Paxs	452.48	Joback Method
dvisc	0.0002559	Paxs	495.93	Joback Method
dvisc	0.0001828	Paxs	539.39	Joback Method
dvisc	0.0001372	Paxs	582.85	Joback Method
dvisc	0.0001072	Paxs	626.31	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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