

Carbonic acid, butyl 4-methoxyphenyl ester

Inchi:	InChI=1S/C12H16O4/c1-3-4-9-15-12(13)16-11-7-5-10(14-2)6-8-11/h5-8H,3-4,9H2,1-2H3
InchiKey:	PMCJWQJCEHBUPE-UHFFFAOYSA-N
Formula:	C12H16O4
SMILES:	CCCCOC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]:	224.25

Physical Properties

Property code	Value	Unit	Source
gf	-290.98	kJ/mol	Joback Method
hf	-575.19	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	59.22	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.011		Crippen Method
mvol	175.360	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinpol	1716.00		NIST Webbook
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tb	626.75	K	Joback Method
tc	829.69	K	Joback Method
tf	380.56	K	Joback Method
vc	0.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.01	J/molxK	626.75	Joback Method
cpg	509.52	J/molxK	795.87	Joback Method
cpg	498.13	J/molxK	762.04	Joback Method
cpg	485.98	J/molxK	728.22	Joback Method
cpg	473.07	J/molxK	694.40	Joback Method
cpg	459.41	J/molxK	660.57	Joback Method
cpg	520.12	J/molxK	829.69	Joback Method
dvisc	0.0001151	Paxs	626.75	Joback Method

dvisc	0.0001446	Paxs	585.72	Joback Method
dvisc	0.0001878	Paxs	544.69	Joback Method
dvisc	0.0002546	Paxs	503.65	Joback Method
dvisc	0.0003643	Paxs	462.62	Joback Method
dvisc	0.0005590	Paxs	421.59	Joback Method
dvisc	0.0009407	Paxs	380.56	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=U357849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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