

Benzoic acid, 3-methoxy-, butyl ester

Inchi:	InChI=1S/C12H16O3/c1-3-4-8-15-12(13)10-6-5-7-11(9-10)14-2/h5-7,9H,3-4,8H2,1-2H3
InchiKey:	BQGRZDUSDFGMHU-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	208.25

Physical Properties

Property code	Value	Unit	Source
gf	-185.98	kJ/mol	Joback Method
hf	-442.97	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	56.81	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.652		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinqol	1632.00		NIST Webbook
tb	604.33	K	Joback Method
tc	809.23	K	Joback Method
tf	358.33	K	Joback Method
vc	0.641	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.31	J/molxK	604.33	Joback Method
cpg	433.95	J/molxK	638.48	Joback Method
cpg	447.83	J/molxK	672.63	Joback Method
cpg	460.95	J/molxK	706.78	Joback Method
cpg	473.32	J/molxK	740.93	Joback Method
cpg	484.93	J/molxK	775.08	Joback Method
cpg	495.80	J/molxK	809.23	Joback Method
dvisc	0.0012736	Paxs	358.33	Joback Method
dvisc	0.0007362	Paxs	399.33	Joback Method

dvisc	0.0004713	Paxs	440.33	Joback Method
dvisc	0.0003255	Paxs	481.33	Joback Method
dvisc	0.0002383	Paxs	522.33	Joback Method
dvisc	0.0001825	Paxs	563.33	Joback Method
dvisc	0.0001450	Paxs	604.33	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=U374513&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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