

Benzoic acid, 3-butyloxy-, methyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H16O3/c1-3-4-8-15-11-7-5-6-10(9-11)12(13)14-2/h5-7,9H,3-4,8H2,1-2H3

FBAGXCNLVAIFMR-UHFFFAOYSA-N

C12H16O3

CCCCOc1cccc(C(=O)OC)c1

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
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	604.33	K	Joback Method
tc	809.23	K	Joback Method
tf	358.33	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.31	J/mol×K	604.33	Joback Method
cpg	433.95	J/mol×K	638.48	Joback Method
cpg	447.83	J/mol×K	672.63	Joback Method
cpg	460.95	J/mol×K	706.78	Joback Method
cpg	473.32	J/mol×K	740.93	Joback Method
cpg	484.93	J/mol×K	775.08	Joback Method
cpg	495.80	J/mol×K	809.23	Joback Method
dvisc	0.0012736	Pa×s	358.33	Joback Method

dvisc	0.0007362	Pa×s	399.33	Joback Method
dvisc	0.0004713	Pa×s	440.33	Joback Method
dvisc	0.0003255	Pa×s	481.33	Joback Method
dvisc	0.0002383	Pa×s	522.33	Joback Method
dvisc	0.0001825	Pa×s	563.33	Joback Method
dvisc	0.0001450	Pa×s	604.33	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=U374500&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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