Benzoic acid, 4-butyl-, methyl ester

Other names:	4-Butylbenzoic acid, methyl ester
	methyl 4-butylbenzoate
Inchi:	InChI=1S/C12H16O2/c1-3-4-5-10-6-8-11(9-7-10)12(13)14-2/h6-9H,3-5H2,1-2H3
InchiKey:	XJRYQLPELPLPHZ-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCCCc1ccc(C(=O)OC)cc1
Mol. weight [g/mol]:	192.25
CAS:	20651-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-80.98	kJ/mol	Joback Method
hf	-310.75	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.816		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1543.00		NIST Webbook
tb	581.91	K	Joback Method
tc	788.90	K	Joback Method
tf	336.10	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.77	J/mol×K	581.91	Joback Method
cpg	460.52	J/mol×K	754.40	Joback Method
cpg	448.71	J/mol×K	719.90	Joback Method
cpg	436.14	J/mol×K	685.41	Joback Method
cpg	422.81	J/mol×K	650.91	Joback Method
cpg	408.69	J/mol×K	616.41	Joback Method

cpg	471.60	J/mol×K	788.90	Joback Method
dvisc	0.0001803	Pa×s	581.91	Joback Method
dvisc	0.0002277	Pa×s	540.94	Joback Method
dvisc	0.0002986	Pa×s	499.97	Joback Method
dvisc	0.0004111	Pa×s	459.00	Joback Method
dvisc	0.0006026	Pa×s	418.04	Joback Method
dvisc	0.0009597	Pa×s	377.07	Joback Method
dvisc	0.0017122	Pa×s	336.10	Joback Method

Sources

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=C20651698&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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