4-Butylbenzoic acid, 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]: 192.26

Physical Properties

Property code	Value	Unit	Source
af	0.6093		Cheméo Relay (1.0)
gf	-80.98	kJ/mol	Joback Method
hf	-365.47	kJ/mol	Cheméo Relay (1.0)
hfus	23.27	kJ/mol	Joback Method
hvap	73.82	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-4.10		Cheméo Relay (1.0)
logp	2.816		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	537.54	K	Cheméo Relay (1.0)
tc	730.80	K	Cheméo Relay (1.0)
tf	271.40	K	Cheméo Relay (1.0)
vc	0.605	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.77	J/mol×K	581.91	Joback Method
cpg	471.60	J/mol×K	788.90	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
dvisc	0.0004111	Pa×s	459.00	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	0.0017122	Pa×s	336.10	Joback Method
dvisc	0.0006026	Pa×s	418.04	Joback Method
dvisc	0.0009597	Pa×s	377.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20651698&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume