Benzoic acid, 4-methoxy-, butyl ester

Other names: n-Butyl anisate
Butyl 4-methoxybenzoate
Inchi: InChI=1S/C12H16O3/c1-3-4-9-15-12(13)10-5-7-11(14-2)8-6-10/h5-8H,3-4,9H2,1-2H3
InchiKey: DXKMHDQQRQRYCI-UHFFFAOYSA-N
Formula: C12H16O3
SMILES: CCCCOC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 208.25
CAS: 6946-35-6

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	1632.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1677.00		NIST Webbook
ripol	2305.00		NIST Webbook
ripol	2305.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6946356&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume