4-Butyloxy-3-methylbenzoic acid, butyl ester

Other names: Butyl 4-butoxy-3-methylbenzoate
Inchi: InChI=1S/C16H24O3/c1-4-6-10-18-15-9-8-14(12-13(15)3)16(17)19-11-7-5-2/h8-9,12H,4-
InchiKey: NSHTUZAELSBODY-UHFFFAOYSA-N
Formula: C16H24O3
SMILES: CCCCOC(=O)c1ccc(OCCCC)c(C)c1
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
gf	-161.93	kJ/mol	Joback Method
hf	-537.00	kJ/mol	Joback Method
hfus	34.43	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.131		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	2032.00		NIST Webbook
tb	700.83	K	Joback Method
tc	896.69	K	Joback Method
tf	415.93	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.88	J/mol×K	700.83	Joback Method
cpg	644.40	J/mol×K	733.47	Joback Method
cpg	660.01	J/mol×K	766.12	Joback Method
cpg	674.73	J/mol×K	798.76	Joback Method
cpg	688.57	J/mol×K	831.40	Joback Method
cpg	701.53	J/mol×K	864.05	Joback Method
cpg	713.61	J/mol×K	896.69	Joback Method
dvisc	0.0008365	Pa×s	415.93	Joback Method

dvisc	0.0004819	Pa×s	463.41	Joback Method
dvisc	0.0003076	Pa×s	510.90	Joback Method
dvisc	0.0002119	Pa×s	558.38	Joback Method
dvisc	0.0001548	Pa×s	605.86	Joback Method
dvisc	0.0001184	Pa×s	653.35	Joback Method
dvisc	0.0000938	Pa×s	700.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378752&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume