4-Butylbenzoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C17H26O3/c1-4-5-6-15-7-9-16(10-8-15)17(18)20-13-14(2)11-12-19-3/h7-10,14

InchiKey: MAPCYJGHNRLAOA-UHFFFAOYSA-N

Formula: C17H26O3

SMILES: CCCCc1ccc(C(=O)OCC(C)CCOC)cc1

Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
gf	-146.32	kJ/mol	Joback Method
hf	-551.45	kJ/mol	Joback Method
hfus	33.89	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.859		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
rinpol	2139.00		NIST Webbook
tb	718.29	K	Joback Method
tc	914.63	K	Joback Method
tf	399.68	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.29	J/mol×K	718.29	Joback Method
cpg	760.77	J/mol×K	881.91	Joback Method
cpg	747.40	J/mol×K	849.18	Joback Method
cpg	733.09	J/mol×K	816.46	Joback Method
cpg	717.81	J/mol×K	783.74	Joback Method
cpg	701.55	J/mol×K	751.01	Joback Method
cpg	773.21	J/mol×K	914.63	Joback Method
dvisc	0.0000770	Pa×s	718.29	Joback Method
dvisc	0.0001008	Pa×s	665.19	Joback Method

dvisc	0.0001382	Pa×s	612.09	Joback Method
dvisc	0.0002012	Pa×s	558.99	Joback Method
dvisc	0.0003171	Pa×s	505.88	Joback Method
dvisc	0.0005559	Pa×s	452.78	Joback Method
dvisc	0.0011313	Pa×s	399.68	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=U354320&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