P-METHOXYPHENYL P-BUTYLBENZOATE

Other names: 4-Butylbenzoic acid, 4-methoxyphenyl ester
Inchi: InChI=1S/C18H20O3/c1-3-4-5-14-6-8-15(9-7-14)18(19)21-17-12-10-16(20-2)11-13-17/h6
InchiKey: BISLKTRYMAGJLH-UHFFFAOYSA-N
Formula: C18H20O3
SMILES: CCCCc1ccc(C(=O)Oc2ccc(OC)cc2)cc1
Mol. weight [g/mol]: 284.35

Physical Properties

Property code	Value	Unit	Source
af	0.8204		Cheméo Relay (1.0)
hf	-390.16	kJ/mol	Cheméo Relay (1.0)
hfus	33.65	kJ/mol	Joback Method
hvap	95.75	kJ/mol	Cheméo Relay (1.0)
ie	7.96	eV	Cheméo Relay (1.0)
log10ws	-5.38		Cheméo Relay (1.0)
logp	4.257		Crippen Method
mcvol	230.270	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2351.00		NIST Webbook
tb	649.78	K	Cheméo Relay (1.0)
tc	875.65	K	Cheméo Relay (1.0)
tf	322.75	K	Cheméo Relay (1.0)
vc	0.846	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.57	J/mol×K	773.27	Joback Method
cpg	730.12	J/mol×K	997.10	Joback Method
cpg	720.04	J/mol×K	959.80	Joback Method
cpg	708.86	J/mol×K	922.49	Joback Method
cpg	696.55	J/mol×K	885.19	Joback Method
cpg	683.08	J/mol×K	847.88	Joback Method
cpg	668.43	J/mol×K	810.58	Joback Method

dvisc	0.0001661	Pa×s	619.08	Joback Method
dvisc	0.0000752	Pa×s	773.27	Joback Method
dvisc	0.0000943	Pa×s	721.87	Joback Method
dvisc	0.0001225	Pa×s	670.48	Joback Method
dvisc	0.0006204	Pa×s	464.89	Joback Method
dvisc	0.0002380	Pa×s	567.68	Joback Method
dvisc	0.0003663	Pa×s	516.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35684232&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume