4-butylbenzoic acid, cyclobutyl ester

Inchi: InChI=1S/C15H20O2/c1-2-3-5-12-8-10-13(11-9-12)15(16)17-14-6-4-7-14/h8-11,14H,2-7H
InchiKey: ZTHKVMBWGQYZRK-UHFFFAOYSA-N
Formula: C15H20O2
SMILES: CCCCc1ccc(C(=O)OC2CCC2)cc1
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
hfus	27.08	kJ/mol	Joback Method
hvap	84.96	kJ/mol	Cheméo Relay (1.0)
ie	9.07	eV	Cheméo Relay (1.0)
logp	3.739		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
rinpol	1857.40		NIST Webbook
rinpol	1857.40		NIST Webbook
tb	595.05	K	Cheméo Relay (1.0)
tf	242.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.87	J/mol×K	661.56	Joback Method
cpg	551.73	J/mol×K	697.80	Joback Method
cpg	568.44	J/mol×K	734.03	Joback Method
cpg	584.05	J/mol×K	770.27	Joback Method
cpg	598.62	J/mol×K	806.51	Joback Method
cpg	612.18	J/mol×K	842.74	Joback Method
cpg	624.79	J/mol×K	878.98	Joback Method
dvisc	0.0017903	Pa×s	384.33	Joback Method
dvisc	0.0010919	Pa×s	430.54	Joback Method
dvisc	0.0007329	Pa×s	476.74	Joback Method
dvisc	0.0005279	Pa×s	522.94	Joback Method
dvisc	0.0004010	Pa×s	569.15	Joback Method
dvisc	0.0003175	Pa×s	615.36	Joback Method

dvisc	0.0002597	Pa×s	661.56	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292205&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point