

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
gf	-7.07	kJ/mol	Joback Method
hf	-306.03	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	61.16	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.739		Crippen Method
mvol	195.030	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1857.40		NIST Webbook
rinpol	1857.40		NIST Webbook
tb	661.56	K	Joback Method
tc	878.98	K	Joback Method
tf	384.33	K	Joback Method
vc	0.741	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.87	J/molxK	661.56	Joback Method
cpg	551.73	J/molxK	697.80	Joback Method
cpg	568.44	J/molxK	734.03	Joback Method
cpg	584.05	J/molxK	770.27	Joback Method
cpg	598.62	J/molxK	806.51	Joback Method
cpg	612.18	J/molxK	842.74	Joback Method
cpg	624.79	J/molxK	878.98	Joback Method
dvisc	0.0017903	Paxs	384.33	Joback Method

dvisc	0.0010919	Paxs	430.54	Joback Method
dvisc	0.0007329	Paxs	476.74	Joback Method
dvisc	0.0005279	Paxs	522.94	Joback Method
dvisc	0.0004010	Paxs	569.15	Joback Method
dvisc	0.0003175	Paxs	615.36	Joback Method
dvisc	0.0002597	Paxs	661.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U292205&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

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