

Butyl 4-acetoxybenzoate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C13H16O4/c1-3-4-9-16-13(15)11-5-7-12(8-6-11)17-10(2)14/h5-8H,3-4,9H2,1-2H

MYCRBPXYIRYAON-UHFFFAOYSA-N

C13H16O4

CCCCOC(=O)c1ccc(OC(C)=O)cc1

236.26

Physical Properties

Property code	Value	Unit	Source
gf	-306.48	kJ/mol	Joback Method
hf	-576.19	kJ/mol	Joback Method
hfus	28.65	kJ/mol	Joback Method
hvap	65.78	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.569		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1767.00		NIST Webbook
rinpol	1767.00		NIST Webbook
tb	681.08	K	Joback Method
tc	889.77	K	Joback Method
tf	419.53	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.57	J/mol×K	681.08	Joback Method
cpg	501.48	J/mol×K	715.86	Joback Method
cpg	514.53	J/mol×K	750.64	Joback Method
cpg	526.74	J/mol×K	785.42	Joback Method
cpg	538.09	J/mol×K	820.20	Joback Method
cpg	548.61	J/mol×K	854.99	Joback Method
cpg	558.29	J/mol×K	889.77	Joback Method
dvisc	0.0010519	Pa×s	419.53	Joback Method

dvisc	0.0006345	Pa×s	463.12	Joback Method
dvisc	0.0004175	Pa×s	506.71	Joback Method
dvisc	0.0002935	Pa×s	550.30	Joback Method
dvisc	0.0002173	Pa×s	593.90	Joback Method
dvisc	0.0001677	Pa×s	637.49	Joback Method
dvisc	0.0001337	Pa×s	681.08	Joback Method

Sources

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=U373006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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