n-Butyl 3,4-dimethoxybenzoate

Other names: Benzoi acid, 3,4-dimethoxy, n-butyl ester
Inchi: InChI=1S/C13H18O4/c1-4-5-8-17-13(14)10-6-7-11(15-2)12(9-10)16-3/h6-7,9H,4-5,8H2,1
InchiKey: ABBWKQQUUQIENF-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: CCCCOC(=O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-292.19	kJ/mol	Joback Method
hf	-607.30	kJ/mol	Joback Method
hfus	27.85	kJ/mol	Joback Method
hvap	62.11	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.661		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1917.00		NIST Webbook
tb	654.61	K	Joback Method
tc	855.69	K	Joback Method
tf	404.35	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.34	J/mol×K	654.61	Joback Method
cpg	510.17	J/mol×K	688.12	Joback Method
cpg	524.25	J/mol×K	721.64	Joback Method
cpg	537.54	J/mol×K	755.15	Joback Method
cpg	550.05	J/mol×K	788.67	Joback Method
cpg	561.75	J/mol×K	822.18	Joback Method
cpg	572.64	J/mol×K	855.69	Joback Method
dvisc	0.0007305	Pa×s	404.35	Joback Method

dvisc	0.0004518	Pa×s	446.06	Joback Method
dvisc	0.0003034	Pa×s	487.77	Joback Method
dvisc	0.0002169	Pa×s	529.48	Joback Method
dvisc	0.0001628	Pa×s	571.19	Joback Method
dvisc	0.0001271	Pa×s	612.90	Joback Method
dvisc	0.0001024	Pa×s	654.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372926&Units=SI
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

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