Butyl 3,4-dimethylbenzoate

Other names: Benzoic acid, 3,4-dimethyl-, n-butyl ester
Inchi: InChI=1S/C13H18O2/c1-4-5-8-15-13(14)12-7-6-10(2)11(3)9-12/h6-7,9H,4-5,8H2,1-3H3
InchiKey: BWZNCIFOYGRWMO-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CCCCOC(=O)c1ccc(C)c(C)c1
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-82.19	kJ/mol	Joback Method
hf	-342.86	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	57.29	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.260		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1587.00		NIST Webbook
tb	609.77	K	Joback Method
tc	814.57	K	Joback Method
tf	359.89	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.69	J/mol×K	609.77	Joback Method
cpg	511.58	J/mol×K	780.44	Joback Method
cpg	499.35	J/mol×K	746.30	Joback Method
cpg	486.36	J/mol×K	712.17	Joback Method
cpg	472.59	J/mol×K	678.04	Joback Method
cpg	458.04	J/mol×K	643.90	Joback Method

cpg	523.06	J/mol×K	814.57	Joback Method
dvisc	0.0001624	Pa×s	609.77	Joback Method
dvisc	0.0002024	Pa×s	568.12	Joback Method
dvisc	0.0002613	Pa×s	526.48	Joback Method
dvisc	0.0003525	Pa×s	484.83	Joback Method
dvisc	0.0005029	Pa×s	443.18	Joback Method
dvisc	0.0007724	Pa×s	401.54	Joback Method
dvisc	0.0013102	Pa×s	359.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373236&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

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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