Benzoic acid, 3,4-dimethyl-, ethyl ester

Other names: Ethyl 3,4-dimethylbenzoate
Inchi: InChI=1S/C11H14O2/c1-4-13-11(12)10-6-5-8(2)9(3)7-10/h5-7H,4H2,1-3H3
InchiKey: GTXUIKILNLXONM-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CCOC(=O)c1ccc(C)c(C)c1
Mol. weight [g/mol]: 178.23
CAS: 33499-44-4

Physical Properties

Property code	Value	Unit	Source
gf	-99.03	kJ/mol	Joback Method
hf	-301.58	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	52.84	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.480		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1385.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1432.00		NIST Webbook
tb	564.01	K	Joback Method
tc	775.37	K	Joback Method
tf	337.35	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.82	J/mol×K	564.01	Joback Method
cpg	359.69	J/mol×K	599.24	Joback Method
cpg	372.86	J/mol×K	634.46	Joback Method
cpg	385.33	J/mol×K	669.69	Joback Method

cpg	397.11	J/mol×K	704.92	Joback Method
cpg	408.21	J/mol×K	740.15	Joback Method
cpg	418.63	J/mol×K	775.37	Joback Method
dvisc	0.0013555	Pa×s	337.35	Joback Method
dvisc	0.0008295	Pa×s	375.13	Joback Method
dvisc	0.0005553	Pa×s	412.90	Joback Method
dvisc	0.0003976	Pa×s	450.68	Joback Method
dvisc	0.0002998	Pa×s	488.46	Joback Method
dvisc	0.0002354	Pa×s	526.23	Joback Method
dvisc	0.0001909	Pa×s	564.01	Joback Method

Sources

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=C33499444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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