Ethyl 4-t-butylbenzoate

Other names: Ethyl 4-tert-butylbenzoate
Benzoic acid, 4-(1,1-dimethylethyl)-, ethyl ester
ethyl 4-(1,1-dimethylethyl)benzoate
Inchi: InChI=1S/C13H18O2/c1-5-15-12(14)10-6-8-11(9-7-10)13(2,3)4/h6-9H,5H2,1-4H3
InchiKey: LIQWHXBLFOERRD-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 206.28
CAS: 5406-57-5

Physical Properties

Property code	Value	Unit	Source
gf	-69.72	kJ/mol	Joback Method
hf	-340.14	kJ/mol	Joback Method
hfus	18.45	kJ/mol	Joback Method
hvap	55.33	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.161		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
tb	601.56	K	Joback Method
tc	817.36	K	Joback Method
tf	349.79	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.22	J/mol×K	601.56	Joback Method
cpg	462.62	J/mol×K	637.53	Joback Method
cpg	477.98	J/mol×K	673.49	Joback Method
cpg	492.35	J/mol×K	709.46	Joback Method

cpg	505.78	J/mol×K	745.43	Joback Method
cpg	518.30	J/mol×K	781.39	Joback Method
cpg	529.96	J/mol×K	817.36	Joback Method
dvisc	0.0018655	Pa×s	349.79	Joback Method
dvisc	0.0009730	Pa×s	391.75	Joback Method
dvisc	0.0005756	Pa×s	433.71	Joback Method
dvisc	0.0003736	Pa×s	475.67	Joback Method
dvisc	0.0002601	Pa×s	517.64	Joback Method
dvisc	0.0001911	Pa×s	559.60	Joback Method
dvisc	0.0001467	Pa×s	601.56	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5406575&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

Latest version available from: