4-Ethylbenzoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C17H18O2/c1-4-14-5-7-15(8-6-14)17(18)19-16-10-12(2)9-13(3)11-16/h5-11H,4
InchiKey: ZMOPANMCRAAXCA-UHFFFAOYSA-N
Formula: C17H18O2
SMILES: CCc1ccc(C(=O)Oc2cc(C)cc(C)c2)cc1
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	54.27	kJ/mol	Joback Method
hf	-200.36	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.085		Crippen Method
mcvol	210.310	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	2075.00		NIST Webbook
rinpol	2075.00		NIST Webbook
tb	732.95	K	Joback Method
tc	963.96	K	Joback Method
tf	443.91	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.53	J/mol×K	732.95	Joback Method
cpg	638.23	J/mol×K	925.46	Joback Method
cpg	626.68	J/mol×K	886.96	Joback Method
cpg	614.07	J/mol×K	848.46	Joback Method
cpg	600.37	J/mol×K	809.95	Joback Method
cpg	585.53	J/mol×K	771.45	Joback Method
cpg	648.76	J/mol×K	963.96	Joback Method
dvisc	0.0001097	Pa×s	732.95	Joback Method

dvisc	0.0001354	Pa×s	684.78	Joback Method
dvisc	0.0001725	Pa×s	636.60	Joback Method
dvisc	0.0002286	Pa×s	588.43	Joback Method
dvisc	0.0003187	Pa×s	540.26	Joback Method
dvisc	0.0004742	Pa×s	492.08	Joback Method
dvisc	0.0007691	Pa×s	443.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307123&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