4-Ethylbenzoic acid, cyclobutyl ester

Inchi: InChI=1S/C13H16O2/c1-2-10-6-8-11(9-7-10)13(14)15-12-4-3-5-12/h6-9,12H,2-5H2,1H3
InchiKey: LZFCLOXJWLIITN-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: CCc1ccc(C(=O)OC2CCC2)cc1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	-23.91	kJ/mol	Joback Method
hf	-264.75	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.958		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1641.20		NIST Webbook
rinpol	1641.20		NIST Webbook
tb	615.80	K	Joback Method
tc	841.18	K	Joback Method
tf	361.79	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.12	J/mol×K	615.80	Joback Method
cpg	447.15	J/mol×K	653.36	Joback Method
cpg	463.06	J/mol×K	690.93	Joback Method
cpg	477.90	J/mol×K	728.49	Joback Method
cpg	491.71	J/mol×K	766.05	Joback Method
cpg	504.53	J/mol×K	803.62	Joback Method
cpg	516.43	J/mol×K	841.18	Joback Method
dvisc	0.0018557	Pa×s	361.79	Joback Method

dvisc	0.0011736	Pa×s	404.12	Joback Method
dvisc	0.0008095	Pa×s	446.46	Joback Method
dvisc	0.0005955	Pa×s	488.79	Joback Method
dvisc	0.0004601	Pa×s	531.13	Joback Method
dvisc	0.0003692	Pa×s	573.46	Joback Method
dvisc	0.0003054	Pa×s	615.80	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=U292196&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