4-Ethylbenzoic acid, cyclopentyl ester

Other names: Cyclopentyl 4-ethylbenzoate
Inchi: InChI=1S/C14H18O2/c1-2-11-7-9-12(10-8-11)14(15)16-13-5-3-4-6-13/h7-10,13H,2-6H2,1
InchiKey: HBTFJMMUGOMQHA-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: CCc1ccc(C(=O)OC2CCCC2)cc1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	-27.59	kJ/mol	Joback Method
hf	-291.55	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	59.11	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.348		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
ripol	1835.00		NIST Webbook
ripol	1835.00		NIST Webbook
tb	642.95	K	Joback Method
tc	871.46	K	Joback Method
tf	369.54	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.33	J/mol×K	642.95	Joback Method
cpg	563.19	J/mol×K	833.37	Joback Method
cpg	549.55	J/mol×K	795.29	Joback Method
cpg	534.78	J/mol×K	757.20	Joback Method
cpg	518.85	J/mol×K	719.12	Joback Method
cpg	501.71	J/mol×K	681.03	Joback Method
cpg	575.77	J/mol×K	871.46	Joback Method

dvisc	0.0002127	Pa×s	642.95	Joback Method
dvisc	0.0002662	Pa×s	597.38	Joback Method
dvisc	0.0003457	Pa×s	551.81	Joback Method
dvisc	0.0004705	Pa×s	506.25	Joback Method
dvisc	0.0006807	Pa×s	460.68	Joback Method
dvisc	0.0010679	Pa×s	415.11	Joback Method
dvisc	0.0018722	Pa×s	369.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U293320&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume