4-Ethylbenzoic acid, pentyl ester

Inchi: InChI=1S/C14H20O2/c1-3-5-6-11-16-14(15)13-9-7-12(4-2)8-10-13/h7-10H,3-6,11H2,1-2
InchiKey: ZQAAPECGIMFVID-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCCCCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	-64.14	kJ/mol	Joback Method
hf	-352.03	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.596		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1717.80		NIST Webbook
rinpol	1717.80		NIST Webbook
tb	627.67	K	Joback Method
tc	828.65	K	Joback Method
tf	358.64	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.85	J/mol×K	627.67	Joback Method
cpg	565.96	J/mol×K	795.15	Joback Method
cpg	553.21	J/mol×K	761.65	Joback Method
cpg	539.64	J/mol×K	728.16	Joback Method
cpg	525.23	J/mol×K	694.66	Joback Method
cpg	509.98	J/mol×K	661.17	Joback Method
cpg	577.93	J/mol×K	828.65	Joback Method
dvisc	0.0001497	Pa×s	627.67	Joback Method

dvisc	0.0001908	Pa×s	582.83	Joback Method
dvisc	0.0002532	Pa×s	537.99	Joback Method
dvisc	0.0003538	Pa×s	493.16	Joback Method
dvisc	0.0005285	Pa×s	448.32	Joback Method
dvisc	0.0008632	Pa×s	403.48	Joback Method
dvisc	0.0015939	Pa×s	358.64	Joback Method

Sources

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=U292342&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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