Benzenepropanoic acid, pentyl ester

Other names: n-Pentyl 3-phenylpropanoate
Inchi: InChI=1S/C14H20O2/c1-2-3-7-12-16-14(15)11-10-13-8-5-4-6-9-13/h4-6,8-9H,2-3,7,10-12
InchiKey: ZCOWYOGEJLZCOM-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCCCCOC(=O)CCc1ccccc1
Mol. weight [g/mol]: 220.31
CAS: 232949-65-4

Physical Properties

Property code	Value	Unit	Source
gf	-54.51	kJ/mol	Joback Method
hf	-340.56	kJ/mol	Joback Method
hfus	28.84	kJ/mol	Joback Method
hvap	58.19	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.353		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1614.00		NIST Webbook
ripol	2185.00		NIST Webbook
tb	622.69	K	Joback Method
tc	822.76	K	Joback Method
tf	346.12	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.13	J/mol×K	622.69	Joback Method
cpg	510.47	J/mol×K	656.04	Joback Method
cpg	525.89	J/mol×K	689.38	Joback Method
cpg	540.43	J/mol×K	722.73	Joback Method
cpg	554.11	J/mol×K	756.07	Joback Method
cpg	566.96	J/mol×K	789.42	Joback Method

cpg	579.01	J/mol×K	822.76	Joback Method
dvisc	0.0020543	Pa×s	346.12	Joback Method
dvisc	0.0010310	Pa×s	392.21	Joback Method
dvisc	0.0005982	Pa×s	438.31	Joback Method
dvisc	0.0003849	Pa×s	484.40	Joback Method
dvisc	0.0002674	Pa×s	530.50	Joback Method
dvisc	0.0001969	Pa×s	576.60	Joback Method
dvisc	0.0001517	Pa×s	622.69	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=C232949654&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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