Benzeneacetic acid, hexyl ester

Other names:	n-Hexyl phenylacetate
	Hexyl phenylacetate
	Phenylacetic acid hexyl ester
Inchi:	InChI=1S/C14H20O2/c1-2-3-4-8-11-16-14(15)12-13-9-6-5-7-10-13/h5-7,9-10H,2-4,8,11-1
InchiKey:	MTAHGWGAEGVCLS-UHFFFAOYSA-N
Formula:	C14H20O2
SMILES:	CCCCCCOC(=O)Cc1ccccc1
Mol. weight [g/mol]:	220.31
CAS:	5421-17-0

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	1605.59		NIST Webbook
rinpol	1627.92		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1605.59		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2148.00		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

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5421170&Units=SI

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