5-Phenylvaleric acid, hexyl ester

Inchi: InChI=1S/C17H26O2/c1-2-3-4-10-15-19-17(18)14-9-8-13-16-11-6-5-7-12-16/h5-7,11-12H
InchiKey: MDGSXKNIPGHYHH-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-29.25	kJ/mol	Joback Method
hf	-402.48	kJ/mol	Joback Method
hfus	36.61	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.523		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	691.33	K	Joback Method
tc	884.75	K	Joback Method
tf	379.93	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.86	J/mol×K	691.33	Joback Method
cpg	672.36	J/mol×K	723.57	Joback Method
cpg	688.87	J/mol×K	755.80	Joback Method
cpg	704.44	J/mol×K	788.04	Joback Method
cpg	719.09	J/mol×K	820.27	Joback Method
cpg	732.85	J/mol×K	852.51	Joback Method
cpg	745.76	J/mol×K	884.75	Joback Method
dvisc	0.0016807	Pa×s	379.93	Joback Method

dvisc	0.0008086	Pa×s	431.83	Joback Method
dvisc	0.0004552	Pa×s	483.73	Joback Method
dvisc	0.0002864	Pa×s	535.63	Joback Method
dvisc	0.0001956	Pa×s	587.53	Joback Method
dvisc	0.0001421	Pa×s	639.43	Joback Method
dvisc	0.0001083	Pa×s	691.33	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=U406075&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume