5-Phenylvaleric acid, pent-2-yl ester

Inchi: InChI=1S/C16H24O2/c1-3-9-14(2)18-16(17)13-8-7-12-15-10-5-4-6-11-15/h4-6,10-11,14H
InchiKey: UZVOMTSKPPMVGR-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: CCCC(C)OC(=O)CCCCc1ccccc1
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	-40.11	kJ/mol	Joback Method
hf	-387.12	kJ/mol	Joback Method
hfus	30.50	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.131		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	668.01	K	Joback Method
tc	866.60	K	Joback Method
tf	353.66	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.45	J/mol×K	668.01	Joback Method
cpg	617.94	J/mol×K	701.11	Joback Method
cpg	634.43	J/mol×K	734.21	Joback Method
cpg	649.95	J/mol×K	767.31	Joback Method
cpg	664.53	J/mol×K	800.40	Joback Method
cpg	678.21	J/mol×K	833.50	Joback Method
cpg	691.01	J/mol×K	866.60	Joback Method
dvisc	0.0022754	Pa×s	353.66	Joback Method

dvisc	0.0009989	Pa×s	406.05	Joback Method
dvisc	0.0005293	Pa×s	458.44	Joback Method
dvisc	0.0003195	Pa×s	510.84	Joback Method
dvisc	0.0002118	Pa×s	563.23	Joback Method
dvisc	0.0001506	Pa×s	615.62	Joback Method
dvisc	0.0001130	Pa×s	668.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406896&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

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