5-Phenylvaleric acid, 4-methyl-2-pentyl ester

Inchi: InChI=1S/C17H26O2/c1-14(2)13-15(3)19-17(18)12-8-7-11-16-9-5-4-6-10-16/h4-6,9-10,1
InchiKey: DVBANFVLFAZSGD-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CC(C)CC(C)OC(=O)CCCCc1ccccc1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-34.13	kJ/mol	Joback Method
hf	-413.04	kJ/mol	Joback Method
hfus	29.57	kJ/mol	Joback Method
hvap	64.09	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.377		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1884.00		NIST Webbook
rinpol	1884.00		NIST Webbook
tb	690.45	K	Joback Method
tc	890.12	K	Joback Method
tf	349.93	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.80	J/mol×K	690.45	Joback Method
cpg	673.91	J/mol×K	723.73	Joback Method
cpg	690.97	J/mol×K	757.01	Joback Method
cpg	706.99	J/mol×K	790.29	Joback Method
cpg	722.02	J/mol×K	823.57	Joback Method
cpg	736.09	J/mol×K	856.85	Joback Method
cpg	749.23	J/mol×K	890.12	Joback Method
dvisc	0.0026892	Pa×s	349.93	Joback Method

dvisc	0.0010374	Pa×s	406.68	Joback Method
dvisc	0.0005053	Pa×s	463.44	Joback Method
dvisc	0.0002880	Pa×s	520.19	Joback Method
dvisc	0.0001833	Pa×s	576.94	Joback Method
dvisc	0.0001265	Pa×s	633.70	Joback Method
dvisc	0.0000928	Pa×s	690.45	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=U406074&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume