5-Phenylvaleric acid, 2-ethylhexyl ester

Inchi: InChI=1S/C19H30O2/c1-3-5-11-17(4-2)16-21-19(20)15-10-9-14-18-12-7-6-8-13-18/h6-8,
InchiKey: SLWMHUHQQGJULD-UHFFFAOYSA-N
Formula: C19H30O2
SMILES: CCCCC(CC)COC(=O)CCCCc1ccccc1
Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	-14.85	kJ/mol	Joback Method
hf	-449.04	kJ/mol	Joback Method
hfus	38.27	kJ/mol	Joback Method
hvap	68.93	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.159		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2113.00		NIST Webbook
rinpol	2113.00		NIST Webbook
tb	736.65	K	Joback Method
tc	930.19	K	Joback Method
tf	387.47	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.54	J/mol×K	736.65	Joback Method
cpg	786.83	J/mol×K	768.91	Joback Method
cpg	804.07	J/mol×K	801.16	Joback Method
cpg	820.28	J/mol×K	833.42	Joback Method
cpg	835.51	J/mol×K	865.68	Joback Method
cpg	849.78	J/mol×K	897.93	Joback Method
cpg	863.14	J/mol×K	930.19	Joback Method
dvisc	0.0017401	Pa×s	387.47	Joback Method

dvisc	0.0007395	Pa×s	445.67	Joback Method
dvisc	0.0003830	Pa×s	503.86	Joback Method
dvisc	0.0002273	Pa×s	562.06	Joback Method
dvisc	0.0001488	Pa×s	620.26	Joback Method
dvisc	0.0001047	Pa×s	678.45	Joback Method
dvisc	0.0000779	Pa×s	736.65	Joback Method

Sources

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=U406897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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