Butyric acid, 4-phenyl-, undecyl ester

Inchi: InChI=1S/C21H34O2/c1-2-3-4-5-6-7-8-9-13-19-23-21(22)18-14-17-20-15-11-10-12-16-20
InchiKey: KPFWOXDSMWLIMK-UHFFFAOYSA-N
Formula: C21H34O2
SMILES: CCCCCCCCCCCOC(=O)CCCc1ccccc1
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	4.43	kJ/mol	Joback Method
hf	-485.04	kJ/mol	Joback Method
hfus	46.97	kJ/mol	Joback Method
hvap	73.77	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.083		Crippen Method
mcvol	290.430	ml/mol	McGowan Method
pc	1225.12	kPa	Joback Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook
tb	782.85	K	Joback Method
tc	973.54	K	Joback Method
tf	425.01	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.32	J/mol×K	782.85	Joback Method
cpg	967.58	J/mol×K	941.76	Joback Method
cpg	953.12	J/mol×K	909.98	Joback Method
cpg	937.70	J/mol×K	878.19	Joback Method
cpg	921.29	J/mol×K	846.41	Joback Method
cpg	903.84	J/mol×K	814.63	Joback Method
cpg	981.13	J/mol×K	973.54	Joback Method
dvisc	0.0000649	Pa×s	782.85	Joback Method

dvisc	0.0000861	Pa×s	723.21	Joback Method
dvisc	0.0001203	Pa×s	663.57	Joback Method
dvisc	0.0001796	Pa×s	603.93	Joback Method
dvisc	0.0002925	Pa×s	544.29	Joback Method
dvisc	0.0005373	Pa×s	484.65	Joback Method
dvisc	0.0011705	Pa×s	425.01	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=U406181&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