Butyric acid, 2-phenyl-, undecyl ester

Inchi: InChI=1S/C21H34O2/c1-3-5-6-7-8-9-10-11-15-18-23-21(22)20(4-2)19-16-13-12-14-17-19
InchiKey: CXFZNNNHJTVGDT-UHFFFAOYSA-N
Formula: C21H34O2
SMILES: CCCCCCCCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	1.99	kJ/mol	Joback Method
hf	-490.32	kJ/mol	Joback Method
hfus	43.45	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	6.254		Crippen Method
mcvol	290.430	ml/mol	McGowan Method
pc	1232.01	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
tb	782.41	K	Joback Method
tc	975.05	K	Joback Method
tf	410.01	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.81	J/mol×K	782.41	Joback Method
cpg	968.74	J/mol×K	942.94	Joback Method
cpg	954.20	J/mol×K	910.84	Joback Method
cpg	938.68	J/mol×K	878.73	Joback Method
cpg	922.13	J/mol×K	846.62	Joback Method
cpg	904.52	J/mol×K	814.52	Joback Method
cpg	982.33	J/mol×K	975.05	Joback Method
dvisc	0.0000597	Pa×s	782.41	Joback Method

dvisc	0.0000806	Pa×s	720.34	Joback Method
dvisc	0.0001152	Pa×s	658.28	Joback Method
dvisc	0.0001773	Pa×s	596.21	Joback Method
dvisc	0.0003016	Pa×s	534.14	Joback Method
dvisc	0.0005902	Pa×s	472.08	Joback Method
dvisc	0.0014151	Pa×s	410.01	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=U406022&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