Butyric acid, 2-phenyl-, undec-2-en-1-yl ester

Inchi: InChI=1S/C21H32O2/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: SREKKSONWDEZGI-RVDMUPIBSA-N
Formula: C21H32O2
SMILES: CCCCCCCCC=CCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	82.21	kJ/mol	Joback Method
hf	-373.10	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	73.34	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	6.030		Crippen Method
mcvol	286.130	ml/mol	McGowan Method
pc	1278.25	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
tb	786.57	K	Joback Method
tc	983.94	K	Joback Method
tf	404.93	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.07	J/mol×K	786.57	Joback Method
cpg	942.07	J/mol×K	951.04	Joback Method
cpg	927.82	J/mol×K	918.15	Joback Method
cpg	912.65	J/mol×K	885.25	Joback Method
cpg	896.50	J/mol×K	852.36	Joback Method
cpg	879.32	J/mol×K	819.46	Joback Method
cpg	955.46	J/mol×K	983.94	Joback Method
dvisc	0.0000518	Pa×s	786.57	Joback Method

dvisc	0.0000701	Pa×s	722.96	Joback Method
dvisc	0.0001006	Pa×s	659.36	Joback Method
dvisc	0.0001558	Pa×s	595.75	Joback Method
dvisc	0.0002681	Pa×s	532.14	Joback Method
dvisc	0.0005343	Pa×s	468.54	Joback Method
dvisc	0.0013227	Pa×s	404.93	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=U406920&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