Butyric acid, 2-phenyl-, oct-3-en-2-yl ester

Inchi: InChI=1S/C18H26O2/c1-4-6-7-9-12-15(3)20-18(19)17(5-2)16-13-10-8-11-14-16/h8-15,17
InchiKey: PRQHFUJYDIPSFX-FMIVXFBMSA-N
Formula: C18H26O2
SMILES: CCCCC=CC(C)OC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 274.40

Physical Properties

Property code	Value	Unit	Source
gf	54.51	kJ/mol	Joback Method
hf	-316.46	kJ/mol	Joback Method
hfus	32.36	kJ/mol	Joback Method
hvap	66.28	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.858		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
tb	717.49	K	Joback Method
tc	921.71	K	Joback Method
tf	356.12	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.78	J/mol×K	717.49	Joback Method
cpg	767.86	J/mol×K	887.68	Joback Method
cpg	754.03	J/mol×K	853.64	Joback Method
cpg	739.26	J/mol×K	819.60	Joback Method
cpg	723.49	J/mol×K	785.56	Joback Method
cpg	706.68	J/mol×K	751.53	Joback Method
cpg	780.81	J/mol×K	921.71	Joback Method
dvisc	0.0000707	Pa×s	717.49	Joback Method

dvisc	0.0000968	Pa×s	657.26	Joback Method
dvisc	0.0001411	Pa×s	597.03	Joback Method
dvisc	0.0002240	Pa×s	536.81	Joback Method
dvisc	0.0003997	Pa×s	476.58	Joback Method
dvisc	0.0008430	Pa×s	416.35	Joback Method
dvisc	0.0022889	Pa×s	356.12	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=U406917&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