Butyric acid, 4-phenyl-, oct-3-en-2-yl ester

Inchi: InChI=1S/C18H26O2/c1-3-4-5-7-11-16(2)20-18(19)15-10-14-17-12-8-6-9-13-17/h6-9,11-
InchiKey: PRMJJYPTAPQRAC-YRNVUSSQSA-N
Formula: C18H26O2
SMILES: CCCCC=CC(C)OC(=O)CCCc1ccccc1
Mol. weight [g/mol]: 274.40

Physical Properties

Property code	Value	Unit	Source
gf	56.95	kJ/mol	Joback Method
hf	-311.18	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.687		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	717.93	K	Joback Method
tc	918.97	K	Joback Method
tf	371.12	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.28	J/mol×K	717.93	Joback Method
cpg	705.89	J/mol×K	751.44	Joback Method
cpg	722.44	J/mol×K	784.94	Joback Method
cpg	737.99	J/mol×K	818.45	Joback Method
cpg	752.59	J/mol×K	851.95	Joback Method
cpg	766.29	J/mol×K	885.46	Joback Method
cpg	779.12	J/mol×K	918.97	Joback Method
dvisc	0.0017879	Pa×s	371.12	Joback Method

dvisc	0.0007422	Pa×s	428.92	Joback Method
dvisc	0.0003797	Pa×s	486.72	Joback Method
dvisc	0.0002239	Pa×s	544.52	Joback Method
dvisc	0.0001462	Pa×s	602.33	Joback Method
dvisc	0.0001028	Pa×s	660.13	Joback Method
dvisc	0.0000765	Pa×s	717.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406985&Units=SI
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

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