Butyric acid, 2-phenyl-, octyl ester

Inchi: InChI=1S/C18H28O2/c1-3-5-6-7-8-12-15-20-18(19)17(4-2)16-13-10-9-11-14-16/h9-11,13
InchiKey: PXXZAMMSLSMIBM-UHFFFAOYSA-N
Formula: C18H28O2
SMILES: CCCCCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 276.41

Physical Properties

Property code	Value	Unit	Source
gf	-23.27	kJ/mol	Joback Method
hf	-428.40	kJ/mol	Joback Method
hfus	35.68	kJ/mol	Joback Method
hvap	66.71	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	5.084		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	713.77	K	Joback Method
tc	908.55	K	Joback Method
tf	376.20	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.39	J/mol×K	713.77	Joback Method
cpg	729.45	J/mol×K	746.23	Joback Method
cpg	746.47	J/mol×K	778.70	Joback Method
cpg	762.49	J/mol×K	811.16	Joback Method
cpg	777.54	J/mol×K	843.62	Joback Method
cpg	791.65	J/mol×K	876.08	Joback Method
cpg	804.86	J/mol×K	908.55	Joback Method
dvisc	0.0019145	Pa×s	376.20	Joback Method

dvisc	0.0008220	Pa×s	432.46	Joback Method
dvisc	0.0004288	Pa×s	488.72	Joback Method
dvisc	0.0002558	Pa×s	544.99	Joback Method
dvisc	0.0001681	Pa×s	601.25	Joback Method
dvisc	0.0001187	Pa×s	657.51	Joback Method
dvisc	0.0000886	Pa×s	713.77	Joback Method

Sources

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=U406019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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