Butyric acid, 2-phenyl-, 2-methylpent-3-yl ester

Inchi: InChI=1S/C16H24O2/c1-5-14(13-10-8-7-9-11-13)16(17)18-15(6-2)12(3)4/h7-12,14-15H,5
InchiKey: HDKNDEMKNGDJSO-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: CCC(C(=O)OC(CC)C(C)C)c1ccccc1
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	-44.99	kJ/mol	Joback Method
hf	-397.68	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	61.48	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.158		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
tb	667.13	K	Joback Method
tc	872.79	K	Joback Method
tf	323.66	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.36	J/mol×K	667.13	Joback Method
cpg	619.54	J/mol×K	701.41	Joback Method
cpg	636.63	J/mol×K	735.68	Joback Method
cpg	652.66	J/mol×K	769.96	Joback Method
cpg	667.66	J/mol×K	804.24	Joback Method
cpg	681.68	J/mol×K	838.51	Joback Method
cpg	694.73	J/mol×K	872.79	Joback Method
dvisc	0.0039719	Pa×s	323.66	Joback Method

dvisc	0.0013449	Pa×s	380.91	Joback Method
dvisc	0.0006044	Pa×s	438.15	Joback Method
dvisc	0.0003267	Pa×s	495.39	Joback Method
dvisc	0.0002006	Pa×s	552.64	Joback Method
dvisc	0.0001350	Pa×s	609.88	Joback Method
dvisc	0.0000972	Pa×s	667.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406855&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

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