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

Inchi: InChI=1S/C15H22O2/c1-5-14(13-9-7-6-8-10-13)15(16)17-12(4)11(2)3/h6-12,14H,5H2,1-4
InchiKey: BYYOPFNWBWBMHY-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCC(C(=O)OC(C)C(C)C)c1ccccc1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-53.41	kJ/mol	Joback Method
hf	-377.04	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	59.25	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.768		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
tb	644.25	K	Joback Method
tc	852.91	K	Joback Method
tf	312.39	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.71	J/mol×K	644.25	Joback Method
cpg	565.56	J/mol×K	679.03	Joback Method
cpg	582.33	J/mol×K	713.80	Joback Method
cpg	598.07	J/mol×K	748.58	Joback Method
cpg	612.79	J/mol×K	783.36	Joback Method
cpg	626.54	J/mol×K	818.14	Joback Method
cpg	639.35	J/mol×K	852.91	Joback Method
dvisc	0.0043870	Pa×s	312.39	Joback Method

dvisc	0.0014933	Pa×s	367.70	Joback Method
dvisc	0.0006738	Pa×s	423.01	Joback Method
dvisc	0.0003655	Pa×s	478.32	Joback Method
dvisc	0.0002250	Pa×s	533.63	Joback Method
dvisc	0.0001518	Pa×s	588.94	Joback Method
dvisc	0.0001095	Pa×s	644.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406854&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