Butyric acid, 2-phenyl-, isobutyl ester

Inchi: InChI=1S/C14H20O2/c1-4-13(12-8-6-5-7-9-12)14(15)16-10-11(2)3/h5-9,11,13H,4,10H2,1
InchiKey: WQXRSCCNMOHJSE-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCC(C(=O)OCC(C)C)c1ccccc1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	-59.39	kJ/mol	Joback Method
hf	-351.12	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.379		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
tb	621.81	K	Joback Method
tc	829.67	K	Joback Method
tf	316.12	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.97	J/mol×K	621.81	Joback Method
cpg	570.55	J/mol×K	795.03	Joback Method
cpg	557.32	J/mol×K	760.38	Joback Method
cpg	543.18	J/mol×K	725.74	Joback Method
cpg	528.09	J/mol×K	691.10	Joback Method
cpg	512.03	J/mol×K	656.45	Joback Method
cpg	582.89	J/mol×K	829.67	Joback Method
dvisc	0.0001317	Pa×s	621.81	Joback Method

dvisc	0.0001782	Pa×s	570.86	Joback Method
dvisc	0.0002558	Pa×s	519.91	Joback Method
dvisc	0.0003972	Pa×s	468.96	Joback Method
dvisc	0.0006866	Pa×s	418.02	Joback Method
dvisc	0.0013815	Pa×s	367.07	Joback Method
dvisc	0.0034830	Pa×s	316.12	Joback Method

Sources

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=U406012&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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