

Butyric acid, 2-phenyl-, isopropyl ester

Inchi:	InChI=1S/C13H18O2/c1-4-12(13(14)15-10(2)3)11-8-6-5-7-9-11/h5-10,12H,4H2,1-3H3
InchiKey:	CNFCIURFRWLFF-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCC(C(=O)OC(C)C)c1ccccc1
Mol. weight [g/mol]:	206.28

Physical Properties

Property code	Value	Unit	Source
gf	-67.81	kJ/mol	Joback Method
hf	-330.48	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	55.19	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.132		Crippen Method
mvol	177.710	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
tb	598.93	K	Joback Method
tc	810.13	K	Joback Method
tf	304.85	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.11	J/molxK	598.93	Joback Method
cpg	460.66	J/molxK	634.13	Joback Method
cpg	476.24	J/molxK	669.33	Joback Method
cpg	490.87	J/molxK	704.53	Joback Method
cpg	504.59	J/molxK	739.73	Joback Method
cpg	517.41	J/molxK	774.93	Joback Method
cpg	529.36	J/molxK	810.13	Joback Method
dvisc	0.0037379	Paxs	304.85	Joback Method

dvisc	0.0014984	Paxs	353.86	Joback Method
dvisc	0.0007503	Paxs	402.88	Joback Method
dvisc	0.0004365	Paxs	451.89	Joback Method
dvisc	0.0002824	Paxs	500.90	Joback Method
dvisc	0.0001974	Paxs	549.92	Joback Method
dvisc	0.0001463	Paxs	598.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U406011&Units=SI

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

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