Propanoic acid, 2-methyl-, phenylmethyl ester

Other names:	Isobutyric acid, benzyl ester
	Benzyl isobutanoate
	Benzyl isobutyrate
	Benzyl 2-methylpropionate
	Benzylester kyseliny isomaselne
Inchi:	InChI=1S/C11H14O2/c1-9(2)11(12)13-8-10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3
InchiKey:	UIKJRDSCEYGECG-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CC(C)C(=O)OCc1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	103-28-6

Physical Properties

Property code	Value	Unit	Source
gf	-82.21	kJ/mol	Joback Method
hf	-283.92	kJ/mol	Joback Method
hfus	17.55	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.386		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1288.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1269.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1771.00		NIST Webbook

tb	553.61	K	Joback Method
tc	767.42	K	Joback Method
tf	297.31	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.73	J/mol×K	553.61	Joback Method
cpg	361.56	J/mol×K	589.25	Joback Method
cpg	375.53	J/mol×K	624.88	Joback Method
cpg	388.67	J/mol×K	660.52	Joback Method
cpg	401.00	J/mol×K	696.15	Joback Method
cpg	412.55	J/mol×K	731.79	Joback Method
cpg	423.32	J/mol×K	767.42	Joback Method
dvisc	0.0030377	Pa×s	297.31	Joback Method
dvisc	0.0014284	Pa×s	340.03	Joback Method
dvisc	0.0007949	Pa×s	382.74	Joback Method
dvisc	0.0004976	Pa×s	425.46	Joback Method
dvisc	0.0003393	Pa×s	468.18	Joback Method
dvisc	0.0002466	Pa×s	510.89	Joback Method
dvisc	0.0001883	Pa×s	553.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103286&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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