

Phenyl isobutyrate

Other names:	Isobutyric acid, phenyl ester Phenyl 2-methylpropanoate Phenyl 2-methylpropionate Propanoic acid, 2-methyl, phenyl ester Phenyl isobutanoate
Inchi:	InChI=1S/C10H12O2/c1-8(2)10(11)12-9-6-4-3-5-7-9/h3-8H,1-2H3
InchiKey:	PIZOACXKIKXRDJ-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(C)C(=O)Oc1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	20279-29-2

Physical Properties

Property code	Value	Unit	Source
gf	-90.63	kJ/mol	Joback Method
hf	-263.28	kJ/mol	Joback Method
hfus	14.96	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.248		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
tb	530.73	K	Joback Method
tc	748.19	K	Joback Method
tf	286.04	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.78	J/mol×K	530.73	Joback Method
cpg	362.77	J/mol×K	711.95	Joback Method

cpg	351.91	J/mol×K	675.70	Joback Method
cpg	340.30	J/mol×K	639.46	Joback Method
cpg	327.92	J/mol×K	603.22	Joback Method
cpg	314.76	J/mol×K	566.97	Joback Method
cpg	372.90	J/mol×K	748.19	Joback Method
dvisc	0.0002037	Pa×s	530.73	Joback Method
dvisc	0.0002656	Pa×s	489.95	Joback Method
dvisc	0.0003634	Pa×s	449.17	Joback Method
dvisc	0.0005294	Pa×s	408.38	Joback Method
dvisc	0.0008382	Pa×s	367.60	Joback Method
dvisc	0.0014883	Pa×s	326.82	Joback Method
dvisc	0.0031130	Pa×s	286.04	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=C20279292&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

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