ISOBUTYL P-HYDROXYBENZOATE

Other names:	Isobutyl p-hydroxybenzoate
	p-Hydroxybenzoic acid iso-butyl ester
	Benzoic acid, 4-hydroxy-, 2-methylpropyl ester
	Benzoic acid, p-hydroxy-, isobutyl ester
	p-Oxybenzoesaureisobutylester
	Isobutylparaben
	Methylpropyl p-hydroxybenzoate
Inchi:	InChI=1S/C11H14O3/c1-8(2)7-14-11(13)9-3-5-10(12)6-4-9/h3-6,8,12H,7H2,1-2H3
InchiKey:	XPJVKCRENWUEJH-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CC(C)COC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	194.23

Physical Properties

Property code	Value	Unit	Source
af	0.6990		Cheméo Relay (1.0)
hf	-527.90	kJ/mol	Cheméo Relay (1.0)
hfus	23.33	kJ/mol	Joback Method
hvap	78.29	kJ/mol	Cheméo Relay (1.0)
ie	8.73	eV	Cheméo Relay (1.0)
log10ws	-2.81		Cheméo Relay (1.0)
logp	2.205		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	1699.00		NIST Webbook
rinpol	1699.00		NIST Webbook
tb	573.03	K	Cheméo Relay (1.0)
tc	762.77	K	Cheméo Relay (1.0)
tf	372.50	K	Cheméo Relay (1.0)
vc	0.554	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	399.03	J/mol×K	634.23	Joback Method
cpg	412.17	J/mol×K	671.55	Joback Method
cpg	424.47	J/mol×K	708.87	Joback Method
cpg	435.99	J/mol×K	746.18	Joback Method
cpg	446.79	J/mol×K	783.50	Joback Method
cpg	456.95	J/mol×K	820.82	Joback Method
cpg	466.52	J/mol×K	858.14	Joback Method
dvisc	0.0009998	Pa×s	409.03	Joback Method
dvisc	0.0004133	Pa×s	446.56	Joback Method
dvisc	0.0001960	Pa×s	484.10	Joback Method
dvisc	0.0001034	Pa×s	521.63	Joback Method
dvisc	0.0000595	Pa×s	559.16	Joback Method
dvisc	0.0000367	Pa×s	596.70	Joback Method
dvisc	0.0000240	Pa×s	634.23	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4247023&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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