

Benzoic acid, 3-hydroxy-, 1-methylpropyl ester

Inchi:	InChI=1S/C11H14O3/c1-3-8(2)14-11(13)9-5-4-6-10(12)7-9/h4-8,12H,3H2,1-2H3
InchiKey:	REMJQYAMROQXID-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCC(C)OC(=O)c1cccc(O)c1
Mol. weight [g/mol]:	194.23

Physical Properties

Property code	Value	Unit	Source
gf	-236.83	kJ/mol	Joback Method
hf	-461.23	kJ/mol	Joback Method
hfus	23.33	kJ/mol	Joback Method
hvap	64.14	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.347		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpola	1640.00		NIST Webbook
tb	634.23	K	Joback Method
tc	858.14	K	Joback Method
tf	409.03	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.03	J/molxK	634.23	Joback Method
cpg	412.17	J/molxK	671.55	Joback Method
cpg	424.47	J/molxK	708.87	Joback Method
cpg	435.99	J/molxK	746.18	Joback Method
cpg	446.79	J/molxK	783.50	Joback Method
cpg	456.95	J/molxK	820.82	Joback Method
cpg	466.52	J/molxK	858.14	Joback Method
dvisc	0.0009998	Paxs	409.03	Joback Method
dvisc	0.0004133	Paxs	446.56	Joback Method

dvisc	0.0001960	Paxs	484.10	Joback Method
dvisc	0.0001034	Paxs	521.63	Joback Method
dvisc	0.0000595	Paxs	559.16	Joback Method
dvisc	0.0000367	Paxs	596.70	Joback Method
dvisc	0.0000240	Paxs	634.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375421&Units=SI
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

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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