

Benzoic acid, 2-(1-methylpropyl)oxy-, methyl ester

Inchi:	InChI=1S/C12H16O3/c1-4-9(2)15-11-8-6-5-7-10(11)12(13)14-3/h5-9H,4H2,1-3H3
InchiKey:	FAUHCYPHSNNHPL-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CCC(C)Oc1ccccc1C(=O)OC
Mol. weight [g/mol]:	208.25

Physical Properties

Property code	Value	Unit	Source
gf	-188.42	kJ/mol	Joback Method
hf	-448.25	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.651		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1496.00		NIST Webbook
tb	603.89	K	Joback Method
tc	812.91	K	Joback Method
tf	343.33	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.73	J/molxK	603.89	Joback Method
cpg	434.72	J/molxK	638.73	Joback Method
cpg	448.90	J/molxK	673.56	Joback Method
cpg	462.28	J/molxK	708.40	Joback Method
cpg	474.87	J/molxK	743.24	Joback Method
cpg	486.66	J/molxK	778.07	Joback Method
cpg	497.67	J/molxK	812.91	Joback Method
dvisc	0.0015703	Paxs	343.33	Joback Method
dvisc	0.0008297	Paxs	386.76	Joback Method

dvisc	0.0004986	Paxs	430.18	Joback Method
dvisc	0.0003290	Paxs	473.61	Joback Method
dvisc	0.0002328	Paxs	517.04	Joback Method
dvisc	0.0001738	Paxs	560.46	Joback Method
dvisc	0.0001353	Paxs	603.89	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=U375334&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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