

Benzoic acid, 4-(1-methylethyl)-, methyl ester

Other names:	Benzoic acid, p-isopropyl-, methyl ester Methyl cumate Methyl p-isopropylbenzoate Methyl 4-isopropylbenzoate 4-Isopropylmethyl benzenecarboxylate Methyl cuminate methyl 4-(1-methylethyl)benzoate
Inchi:	InChI=1S/C11H14O2/c1-8(2)9-4-6-10(7-5-9)11(12)13-3/h4-8H,1-3H3
InchiKey:	IPIVTJSCIHXKOE-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	COC(=O)c1ccc(C(C)C)cc1
Mol. weight [g/mol]:	178.23
CAS:	20185-55-1

Physical Properties

Property code	Value	Unit	Source
gf	-91.84	kJ/mol	Joback Method
hf	-295.39	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	51.79	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.597		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	558.59	K	Joback Method
tc	773.47	K	Joback Method
tf	309.83	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.51	J/mol×K	558.59	Joback Method
cpg	411.28	J/mol×K	737.66	Joback Method

cpg	399.87	J/mol×K	701.84	Joback Method
cpg	387.70	J/mol×K	666.03	Joback Method
cpg	374.76	J/mol×K	630.22	Joback Method
cpg	361.03	J/mol×K	594.40	Joback Method
cpg	421.95	J/mol×K	773.47	Joback Method
dvisc	0.0001834	Pa×s	558.59	Joback Method
dvisc	0.0002352	Pa×s	517.13	Joback Method
dvisc	0.0003151	Pa×s	475.67	Joback Method
dvisc	0.0004464	Pa×s	434.21	Joback Method
dvisc	0.0006805	Pa×s	392.75	Joback Method
dvisc	0.0011460	Pa×s	351.29	Joback Method
dvisc	0.0022187	Pa×s	309.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20185551&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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