Benzoic acid, 2-isopropylphenyl ester

Inchi: InChI=1S/C16H16O2/c1-12(2)14-10-6-7-11-15(14)18-16(17)13-8-4-3-5-9-13/h3-12H,1-2H
InchiKey: HRHFLGLKSCJDDM-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: CC(C)c1ccccc1OC(=O)c1ccccc1
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	62.67	kJ/mol	Joback Method
hf	-162.06	kJ/mol	Joback Method
hfus	24.15	kJ/mol	Joback Method
hvap	65.19	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.029		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
tb	699.67	K	Joback Method
tc	938.10	K	Joback Method
tf	392.60	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.51	J/mol×K	699.67	Joback Method
cpg	534.83	J/mol×K	739.41	Joback Method
cpg	549.87	J/mol×K	779.15	Joback Method
cpg	563.70	J/mol×K	818.89	Joback Method
cpg	576.36	J/mol×K	858.62	Joback Method
cpg	587.91	J/mol×K	898.36	Joback Method
cpg	598.40	J/mol×K	938.10	Joback Method
dvisc	0.0013783	Pa×s	392.60	Joback Method

dvisc	0.0007141	Pa×s	443.78	Joback Method
dvisc	0.0004239	Pa×s	494.96	Joback Method
dvisc	0.0002774	Pa×s	546.13	Joback Method
dvisc	0.0001953	Pa×s	597.31	Joback Method
dvisc	0.0001453	Pa×s	648.49	Joback Method
dvisc	0.0001128	Pa×s	699.67	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=U368960&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