

Benzoic acid, 4-isopropyl phenyl ester

Inchi:	InChI=1S/C16H16O2/c1-12(2)13-8-10-15(11-9-13)18-16(17)14-6-4-3-5-7-14/h3-12H,1-2H
InchiKey:	KPVUCQCHICRYHH-UHFFFAOYSA-N
Formula:	C16H16O2
SMILES:	CC(C)c1ccc(OC(=O)c2ccccc2)cc1
Mol. weight [g/mol]:	240.30
CAS:	13936-99-7

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
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/molxK	699.67	Joback Method
cpg	534.83	J/molxK	739.41	Joback Method
cpg	549.87	J/molxK	779.15	Joback Method
cpg	563.70	J/molxK	818.89	Joback Method
cpg	576.36	J/molxK	858.62	Joback Method
cpg	587.91	J/molxK	898.36	Joback Method
cpg	598.40	J/molxK	938.10	Joback Method
dvisc	0.0013783	Paxs	392.60	Joback Method
dvisc	0.0007141	Paxs	443.78	Joback Method

dvisc	0.0004239	Paxs	494.96	Joback Method
dvisc	0.0002774	Paxs	546.13	Joback Method
dvisc	0.0001953	Paxs	597.31	Joback Method
dvisc	0.0001453	Paxs	648.49	Joback Method
dvisc	0.0001128	Paxs	699.67	Joback Method

Sources

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=C13936997&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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