

Isopropyl 4-acetoxybenzoate

Inchi:	InChI=1S/C12H14O4/c1-8(2)15-12(14)10-4-6-11(7-5-10)16-9(3)13/h4-8H,1-3H3
InchiKey:	PUUGJQYFLLDSOH-UHFFFAOYSA-N
Formula:	C12H14O4
SMILES:	CC(=O)Oc1ccc(C(=O)OC(C)C)cc1
Mol. weight [g/mol]:	222.24

Physical Properties

Property code	Value	Unit	Source
gf	-317.34	kJ/mol	Joback Method
hf	-560.83	kJ/mol	Joback Method
hfus	22.54	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.177		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1631.00		NIST Webbook
tb	657.76	K	Joback Method
tc	873.64	K	Joback Method
tf	393.26	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.03	J/molxK	657.76	Joback Method
cpg	450.66	J/molxK	693.74	Joback Method
cpg	463.45	J/molxK	729.72	Joback Method
cpg	475.39	J/molxK	765.70	Joback Method
cpg	486.48	J/molxK	801.68	Joback Method
cpg	496.72	J/molxK	837.66	Joback Method
cpg	506.12	J/molxK	873.64	Joback Method
dvisc	0.0013098	Paxs	393.26	Joback Method
dvisc	0.0007459	Paxs	437.34	Joback Method

dvisc	0.0004709	Paxs	481.43	Joback Method
dvisc	0.0003211	Paxs	525.51	Joback Method
dvisc	0.0002323	Paxs	569.59	Joback Method
dvisc	0.0001761	Paxs	613.68	Joback Method
dvisc	0.0001386	Paxs	657.76	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372945&Units=SI

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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