2-Methoxybenzoic acid anhydride

Inchi: InChI=1S/C16H14O5/c1-19-13-9-5-3-7-11(13)15(17)21-16(18)12-8-4-6-10-14(12)20-2/h3
InchiKey: CPPYQMZQDONVGK-UHFFFAOYSA-N
Formula: C16H14O5
SMILES: COc1ccccc1C(=O)OC(=O)c1ccccc1OC
Mol. weight [g/mol]: 286.28

Physical Properties

Property code	Value	Unit	Source
gf	-283.44	kJ/mol	Joback Method
hf	-545.27	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	77.81	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.701		Crippen Method
mcvol	209.530	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	2379.00		NIST Webbook
tb	803.80	K	Joback Method
tc	1037.51	K	Joback Method
tf	514.51	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.87	J/mol×K	803.80	Joback Method
cpg	634.92	J/mol×K	998.56	Joback Method
cpg	627.00	J/mol×K	959.61	Joback Method
cpg	617.83	J/mol×K	920.65	Joback Method
cpg	607.42	J/mol×K	881.70	Joback Method
cpg	595.77	J/mol×K	842.75	Joback Method
cpg	641.59	J/mol×K	1037.51	Joback Method
dvisc	0.0000730	Pa×s	803.80	Joback Method
dvisc	0.0000901	Pa×s	755.59	Joback Method

dvisc	0.0001143	Pa×s	707.37	Joback Method
dvisc	0.0001501	Pa×s	659.15	Joback Method
dvisc	0.0002060	Pa×s	610.94	Joback Method
dvisc	0.0002982	Pa×s	562.73	Joback Method
dvisc	0.0004629	Pa×s	514.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375011&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

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