

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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.87	J/molxK	803.80	Joback Method
cpg	595.77	J/molxK	842.75	Joback Method
cpg	607.42	J/molxK	881.70	Joback Method
cpg	617.83	J/molxK	920.65	Joback Method
cpg	627.00	J/molxK	959.61	Joback Method
cpg	634.92	J/molxK	998.56	Joback Method
cpg	641.59	J/molxK	1037.51	Joback Method
dvisc	0.0004629	Paxs	514.51	Joback Method
dvisc	0.0002982	Paxs	562.73	Joback Method

dvisc	0.0002060	Paxs	610.94	Joback Method
dvisc	0.0001501	Paxs	659.15	Joback Method
dvisc	0.0001143	Paxs	707.37	Joback Method
dvisc	0.0000901	Paxs	755.59	Joback Method
dvisc	0.0000730	Paxs	803.80	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

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