4-Methylbenzoic acid anhydride

Inchi: InChI=1S/C16H14O3/c1-11-3-7-13(8-4-11)15(17)19-16(18)14-9-5-12(2)6-10-14/h3-10H,1
InchiKey: BJMLLSSSTGHJJE-UHFFFAOYSA-N
Formula: C16H14O3
SMILES: Cc1ccc(C(=O)OC(=O)c2ccc(C)cc2)cc1
Mol. weight [g/mol]: 254.28
CAS: 13222-85-0

Physical Properties

Property code	Value	Unit	Source
chs	-7776.00 ± 7.90	kJ/mol	NIST Webbook
gf	-73.44	kJ/mol	Joback Method
hf	-280.83	kJ/mol	Joback Method
hfs	-521.00 ± 7.90	kJ/mol	NIST Webbook
hfus	28.89	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.301		Crippen Method
mcvol	197.790	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	758.96	K	Joback Method
tc	998.86	K	Joback Method
tf	470.05	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.45	J/mol×K	758.96	Joback Method
cpg	589.55	J/mol×K	958.87	Joback Method
cpg	580.13	J/mol×K	918.89	Joback Method
cpg	569.64	J/mol×K	878.91	Joback Method
cpg	558.06	J/mol×K	838.93	Joback Method
cpg	545.35	J/mol×K	798.94	Joback Method
cpg	597.96	J/mol×K	998.86	Joback Method

dvisc	0.0001235	Pa×s	758.96	Joback Method
dvisc	0.0001530	Pa×s	710.81	Joback Method
dvisc	0.0001955	Pa×s	662.66	Joback Method
dvisc	0.0002595	Pa×s	614.50	Joback Method
dvisc	0.0003615	Pa×s	566.35	Joback Method
dvisc	0.0005355	Pa×s	518.20	Joback Method
dvisc	0.0008599	Pa×s	470.05	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=C13222850&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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