

2-Methylbenzoic acid anhydride

Other names:	2-Methylbenzoic acid anhydride
Inchi:	InChI=1S/C16H14O3/c1-11-7-3-5-9-13(11)15(17)19-16(18)14-10-6-4-8-12(14)2/h3-10H,1
InchiKey:	YLBSXJWDERHYFY-UHFFFAOYSA-N
Formula:	C16H14O3
SMILES:	Cc1cccc1C(=O)OC(=O)c1cccc1C
Mol. weight [g/mol]:	254.29

Physical Properties

Property code	Value	Unit	Source
af	0.6964		Cheméo Relay (1.0)
chs	-7763.40 ± 7.90	kJ/mol	NIST Webbook
gf	-73.44	kJ/mol	Joback Method
hf	-386.95	kJ/mol	Cheméo Relay (1.0)
hfs	-533.50 ± 7.90	kJ/mol	NIST Webbook
hfus	28.89	kJ/mol	Joback Method
hvap	93.39	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-4.06		Cheméo Relay (1.0)
logp	3.301		Crippen Method
mcvol	197.790	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	614.43	K	Cheméo Relay (1.0)
tc	882.87	K	Cheméo Relay (1.0)
tf	327.02	K	Cheméo Relay (1.0)
vc	0.727	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	589.55	J/mol×K	958.87	Joback Method
cpg	597.96	J/mol×K	998.86	Joback Method
dvisc	0.0008599	Pa×s	470.05	Joback Method
dvisc	0.0005355	Pa×s	518.20	Joback Method
dvisc	0.0003615	Pa×s	566.35	Joback Method
dvisc	0.0002595	Pa×s	614.50	Joback Method
dvisc	0.0001955	Pa×s	662.66	Joback Method
dvisc	0.0001530	Pa×s	710.81	Joback Method
dvisc	0.0001235	Pa×s	758.96	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C607863&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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