Aspirin methyl ester

Other names:	Benzoic acid, 2-(acetyloxy)-, methyl ester
	Salicylic acid acetate, methyl ester
	Methyl acetylsalicylate
	Methyl aspirin
	Methyl o-acetoxybenzoate
	Methyl rhodin
	Methyl O-acetylsalicylate
	Methylrhodine
	Acetylsalicylic acid methyl ester
	O-Acetyl methyl salicylate
	NSC 403847
	Salicylic acid, methyl ester, acetate
	Methyl salicylate, O-acetyl-
	Methyl 2-(acetyloxy)benzoate
Inchi:	InChI=1S/C10H10O4/c1-7(11)14-9-6-4-3-5-8(9)10(12)13-2/h3-6H,1-2H3
InchiKey:	ONWPLBKWMAUFGZ-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	COC(=O)c1ccccc1OC(C)=O
Mol. weight [g/mol]:	194.18
CAS:	580-02-9

Physical Properties

Property code	Value	Unit	Source
gf	-331.74	kJ/mol	Joback Method
hf	-514.27	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	59.10	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.398		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1454.00		NIST Webbook
rinpol	1454.00		NIST Webbook
tb	612.44	K	Joback Method
tc	831.50	K	Joback Method
tf	385.72	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.80	J/mol×K	612.44	Joback Method
cpg	391.31	J/mol×K	794.99	Joback Method
cpg	382.23	J/mol×K	758.48	Joback Method
cpg	372.43	J/mol×K	721.97	Joback Method
cpg	361.93	J/mol×K	685.46	Joback Method
cpg	350.71	J/mol×K	648.95	Joback Method
cpg	399.66	J/mol×K	831.50	Joback Method
dvisc	0.0001824	Pa×s	612.44	Joback Method
dvisc	0.0002254	Pa×s	574.65	Joback Method
dvisc	0.0002869	Pa×s	536.87	Joback Method
dvisc	0.0003788	Pa×s	499.08	Joback Method
dvisc	0.0005235	Pa×s	461.29	Joback Method
dvisc	0.0007664	Pa×s	423.51	Joback Method
dvisc	0.0012091	Pa×s	385.72	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C580029&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