

2-Methoxybenzoic acetic anhydride

Inchi:	InChI=1S/C10H10O4/c1-7(11)14-10(12)8-5-3-4-6-9(8)13-2/h3-6H,1-2H3
InchiKey:	AGCGXUFEZFXWRN-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	COc1ccccc1C(=O)OC(C)=O
Mol. weight [g/mol]:	194.18

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	1533.00		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/molxK	612.44	Joback Method
cpg	391.31	J/molxK	794.99	Joback Method
cpg	382.23	J/molxK	758.48	Joback Method
cpg	372.43	J/molxK	721.97	Joback Method
cpg	361.93	J/molxK	685.46	Joback Method
cpg	350.71	J/molxK	648.95	Joback Method
cpg	399.66	J/molxK	831.50	Joback Method
dvisc	0.0001824	Paxs	612.44	Joback Method
dvisc	0.0002254	Paxs	574.65	Joback Method

dvisc	0.0002869	Paxs	536.87	Joback Method
dvisc	0.0003788	Paxs	499.08	Joback Method
dvisc	0.0005235	Paxs	461.29	Joback Method
dvisc	0.0007664	Paxs	423.51	Joback Method
dvisc	0.0012091	Paxs	385.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U375003&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

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