Carbomethox)-salicylic acid, methyl ester

Inchi: InChI=1S/C10H10O5/c1-13-9(11)7-5-3-4-6-8(7)15-10(12)14-2/h3-6H,1-2H3
InchiKey: ZTUQPXFCZFUTTO-UHFFFAOYSA-N
Formula: C10H10O5
SMILES: COC(=O)Oc1ccccc1C(=O)OC
Mol. weight [g/mol]: 210.18

Physical Properties

Property code	Value	Unit	Source
gf	-436.74	kJ/mol	Joback Method
hf	-646.49	kJ/mol	Joback Method
hfus	22.07	kJ/mol	Joback Method
hvap	61.51	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.618		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
tb	634.86	K	Joback Method
tc	851.27	K	Joback Method
tf	407.95	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.29	J/mol×K	634.86	Joback Method
cpg	374.06	J/mol×K	670.93	Joback Method
cpg	385.14	J/mol×K	707.00	Joback Method
cpg	395.52	J/mol×K	743.06	Joback Method
cpg	405.17	J/mol×K	779.13	Joback Method
cpg	414.08	J/mol×K	815.20	Joback Method
cpg	422.22	J/mol×K	851.27	Joback Method
dvisc	0.0009084	Pa×s	407.95	Joback Method

dvisc	0.0005878	Pa×s	445.77	Joback Method
dvisc	0.0004072	Pa×s	483.59	Joback Method
dvisc	0.0002975	Pa×s	521.40	Joback Method
dvisc	0.0002268	Pa×s	559.22	Joback Method
dvisc	0.0001789	Pa×s	597.04	Joback Method
dvisc	0.0001452	Pa×s	634.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374803&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