

2,4,5-Trimethoxy-styrene

Inchi:	InChI=1S/C11H14O3/c1-5-8-6-10(13-3)11(14-4)7-9(8)12-2/h5-7H,1H2,2-4H3
InchiKey:	DAINMNHDGRVBQF-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	C=Cc1cc(OC)c(OC)cc1OC
Mol. weight [g/mol]:	194.23
CAS:	17598-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-101.90	kJ/mol	Joback Method
hf	-339.48	kJ/mol	Joback Method
hfus	19.40	kJ/mol	Joback Method
hvap	50.90	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.355		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	556.64	K	Joback Method
tc	760.91	K	Joback Method
tf	342.64	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.78	J/mol×K	556.64	Joback Method
cpg	418.98	J/mol×K	726.87	Joback Method
cpg	407.68	J/mol×K	692.82	Joback Method
cpg	395.79	J/mol×K	658.78	Joback Method
cpg	383.33	J/mol×K	624.73	Joback Method
cpg	370.32	J/mol×K	590.69	Joback Method
cpg	429.67	J/mol×K	760.91	Joback Method

dvisc	0.0001184	Pa×s	556.64	Joback Method
dvisc	0.0001428	Pa×s	520.97	Joback Method
dvisc	0.0001771	Pa×s	485.31	Joback Method
dvisc	0.0002274	Pa×s	449.64	Joback Method
dvisc	0.0003046	Pa×s	413.97	Joback Method
dvisc	0.0004313	Pa×s	378.31	Joback Method
dvisc	0.0006565	Pa×s	342.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17598037&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

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