o-Anisic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C11H11ClO3/c1-14-10-6-3-2-5-9(10)11(13)15-8-4-7-12/h2-7H,8H2,1H3/b7-4+
InchiKey: WBWAKPXHPTXRTF-QPJJXVBHSA-N
Formula: C11H11ClO3
SMILES: COc1ccccc1C(=O)OCC=CCl
Mol. weight [g/mol]: 226.66

Physical Properties

Property code	Value	Unit	Source
gf	-126.11	kJ/mol	Joback Method
hf	-320.85	kJ/mol	Joback Method
hfus	26.27	kJ/mol	Joback Method
hvap	58.93	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.604		Crippen Method
mcvol	163.340	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	623.04	K	Joback Method
tc	843.89	K	Joback Method
tf	371.90	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.97	J/mol×K	623.04	Joback Method
cpg	430.65	J/mol×K	807.08	Joback Method
cpg	421.20	J/mol×K	770.27	Joback Method
cpg	411.03	J/mol×K	733.47	Joback Method
cpg	400.11	J/mol×K	696.66	Joback Method
cpg	388.43	J/mol×K	659.85	Joback Method
cpg	439.39	J/mol×K	843.89	Joback Method
dvisc	0.0001304	Pa×s	623.04	Joback Method

dvisc	0.0001637	Pa×s	581.18	Joback Method
dvisc	0.0002129	Pa×s	539.33	Joback Method
dvisc	0.0002893	Pa×s	497.47	Joback Method
dvisc	0.0004160	Pa×s	455.61	Joback Method
dvisc	0.0006437	Pa×s	413.76	Joback Method
dvisc	0.0010989	Pa×s	371.90	Joback Method

Sources

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=U292580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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