

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

Inchi:	InChI=1S/C11H11ClO3/c1-14-10-5-3-9(4-6-10)11(13)15-8-2-7-12/h2-7H,8H2,1H3/b7-2+
InchiKey:	TXUYHADQUJYBNC-FARCUNLSSA-N
Formula:	C11H11ClO3
SMILES:	COc1ccc(C(=O)OCC=C(Cl)cc1
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
rinsol	1740.00		NIST Webbook
tb	623.04	K	Joback Method
tc	843.89	K	Joback Method
tf	371.90	K	Joback Method
vc	0.615	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.97	J/molxK	623.04	Joback Method
cpg	388.43	J/molxK	659.85	Joback Method
cpg	400.11	J/molxK	696.66	Joback Method
cpg	411.03	J/molxK	733.47	Joback Method
cpg	421.20	J/molxK	770.27	Joback Method
cpg	430.65	J/molxK	807.08	Joback Method
cpg	439.39	J/molxK	843.89	Joback Method
dvisc	0.0010989	Paxs	371.90	Joback Method
dvisc	0.0006437	Paxs	413.76	Joback Method

dvisc	0.0004160	Paxs	455.61	Joback Method
dvisc	0.0002893	Paxs	497.47	Joback Method
dvisc	0.0002129	Paxs	539.33	Joback Method
dvisc	0.0001637	Paxs	581.18	Joback Method
dvisc	0.0001304	Paxs	623.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299201&Units=SI
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

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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