

m-Toluic acid, 3-chloroprop-2-enyl ester

Other names:	m-toluylic acid, 3-chloroprop-2-enyl ester
Inchi:	InChI=1S/C11H11ClO2/c1-9-4-2-5-10(8-9)11(13)14-7-3-6-12/h2-6,8H,7H2,1H3/b6-3+
InchiKey:	MBSMOYXJNIUOJL-ZZXXKWWIFSA-N
Formula:	C11H11ClO2
SMILES:	<chem>Cc1cccc(C(=O)OCC=CCl)c1</chem>
Mol. weight [g/mol]:	210.66

Physical Properties

Property code	Value	Unit	Source
gf	-21.11	kJ/mol	Joback Method
hf	-188.63	kJ/mol	Joback Method
hfus	25.08	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.904		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1624.10		NIST Webbook
tb	600.62	K	Joback Method
tc	824.35	K	Joback Method
tf	349.67	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.29	J/molxK	600.62	Joback Method
cpg	407.80	J/molxK	787.06	Joback Method
cpg	398.21	J/molxK	749.77	Joback Method
cpg	387.90	J/molxK	712.49	Joback Method
cpg	376.83	J/molxK	675.20	Joback Method
cpg	364.97	J/molxK	637.91	Joback Method
cpg	416.70	J/molxK	824.35	Joback Method
dvisc	0.0001637	Paxs	600.62	Joback Method

dvisc	0.0002060	Paxs	558.79	Joback Method
dvisc	0.0002691	Paxs	516.97	Joback Method
dvisc	0.0003684	Paxs	475.14	Joback Method
dvisc	0.0005358	Paxs	433.32	Joback Method
dvisc	0.0008442	Paxs	391.50	Joback Method
dvisc	0.0014831	Paxs	349.67	Joback Method

Sources

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=U292500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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