4-Ethylbenzoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C12H13ClO2/c1-2-10-4-6-11(7-5-10)12(14)15-9-3-8-13/h3-8H,2,9H2,1H3/b8-3
InchiKey: SJAFWAMUNZHDSD-FPYGCLRLSA-N
Formula: C12H13ClO2
SMILES: CCc1ccc(C(=O)OCC=CCl)cc1
Mol. weight [g/mol]: 224.68

Physical Properties

Property code	Value	Unit	Source
gf	-12.69	kJ/mol	Joback Method
hf	-209.27	kJ/mol	Joback Method
hfus	27.67	kJ/mol	Joback Method
hvap	58.74	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.158		Crippen Method
mcvol	171.560	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1733.10		NIST Webbook
tb	623.50	K	Joback Method
tc	843.18	K	Joback Method
tf	360.94	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.23	J/mol×K	623.50	Joback Method
cpg	413.65	J/mol×K	660.11	Joback Method
cpg	426.21	J/mol×K	696.73	Joback Method
cpg	437.95	J/mol×K	733.34	Joback Method
cpg	448.90	J/mol×K	769.95	Joback Method
cpg	459.11	J/mol×K	806.56	Joback Method
cpg	468.60	J/mol×K	843.18	Joback Method
dvisc	0.0014273	Pa×s	360.94	Joback Method
dvisc	0.0007986	Pa×s	404.70	Joback Method

dvisc	0.0005004	Pa×s	448.46	Joback Method
dvisc	0.0003408	Pa×s	492.22	Joback Method
dvisc	0.0002471	Pa×s	535.98	Joback Method
dvisc	0.0001881	Pa×s	579.74	Joback Method
dvisc	0.0001487	Pa×s	623.50	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292550&Units=SI

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