Acetic acid, 2-propylphenyl ester

Inchi: InChI=1S/C11H14O2/c1-3-6-10-7-4-5-8-11(10)13-9(2)12/h4-5,7-8H,3,6H2,1-2H3
InchiKey: RKMMUVDOPJRSKW-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CCCc1ccccc1OC(C)=O
Mol. weight [g/mol]: 178.23
CAS: 35922-83-9

Physical Properties

Property code	Value	Unit	Source
gf	-89.40	kJ/mol	Joback Method
hf	-290.11	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	52.17	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.564		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1311.00		NIST Webbook
rinpol	1311.00		NIST Webbook
tb	559.03	K	Joback Method
tc	769.35	K	Joback Method
tf	324.83	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.15	J/mol×K	559.03	Joback Method
cpg	360.31	J/mol×K	594.08	Joback Method
cpg	373.70	J/mol×K	629.14	Joback Method
cpg	386.36	J/mol×K	664.19	Joback Method
cpg	398.29	J/mol×K	699.24	Joback Method
cpg	409.50	J/mol×K	734.30	Joback Method
cpg	420.01	J/mol×K	769.35	Joback Method

dvisc	0.0017437	Pa×s	324.83	Joback Method
dvisc	0.0009957	Pa×s	363.86	Joback Method
dvisc	0.0006338	Pa×s	402.90	Joback Method
dvisc	0.0004369	Pa×s	441.93	Joback Method
dvisc	0.0003200	Pa×s	480.96	Joback Method
dvisc	0.0002455	Pa×s	520.00	Joback Method
dvisc	0.0001955	Pa×s	559.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35922839&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