Propionic acid, 2-propylphenyl ester

Inchi: InChI=1S/C12H16O2/c1-3-7-10-8-5-6-9-11(10)14-12(13)4-2/h5-6,8-9H,3-4,7H2,1-2H3
InchiKey: OYEWJLFZKKNYFL-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: CCCc1ccccc1OC(=O)CC
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	-80.98	kJ/mol	Joback Method
hf	-310.75	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.954		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1394.00		NIST Webbook
tb	581.91	K	Joback Method
tc	788.90	K	Joback Method
tf	336.10	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.77	J/mol×K	581.91	Joback Method
cpg	460.52	J/mol×K	754.40	Joback Method
cpg	448.71	J/mol×K	719.90	Joback Method
cpg	436.14	J/mol×K	685.41	Joback Method
cpg	422.81	J/mol×K	650.91	Joback Method
cpg	408.69	J/mol×K	616.41	Joback Method
cpg	471.60	J/mol×K	788.90	Joback Method
dvisc	0.0001803	Pa×s	581.91	Joback Method
dvisc	0.0002277	Pa×s	540.94	Joback Method

dvisc	0.0002986	Pa×s	499.97	Joback Method
dvisc	0.0004111	Pa×s	459.00	Joback Method
dvisc	0.0006026	Pa×s	418.04	Joback Method
dvisc	0.0009597	Pa×s	377.07	Joback Method
dvisc	0.0017122	Pa×s	336.10	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=U360697&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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