Isobutyric acid, 2-propylphenyl ester

Inchi: InChI=1S/C13H18O2/c1-4-7-11-8-5-6-9-12(11)15-13(14)10(2)3/h5-6,8-10H,4,7H2,1-3H3
InchiKey: WUODIVZJEXMCLC-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CCCc1ccccc1OC(=O)C(C)C
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-75.00	kJ/mol	Joback Method
hf	-336.67	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	56.24	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.200		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1460.00		NIST Webbook
tb	604.35	K	Joback Method
tc	812.28	K	Joback Method
tf	332.37	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.45	J/mol×K	604.35	Joback Method
cpg	514.48	J/mol×K	777.63	Joback Method
cpg	501.96	J/mol×K	742.97	Joback Method
cpg	488.62	J/mol×K	708.32	Joback Method
cpg	474.43	J/mol×K	673.66	Joback Method
cpg	459.38	J/mol×K	639.01	Joback Method
cpg	526.19	J/mol×K	812.28	Joback Method
dvisc	0.0001539	Pa×s	604.35	Joback Method
dvisc	0.0001992	Pa×s	559.02	Joback Method

dvisc	0.0002698	Pa×s	513.69	Joback Method
dvisc	0.0003877	Pa×s	468.36	Joback Method
dvisc	0.0006019	Pa×s	423.03	Joback Method
dvisc	0.0010385	Pa×s	377.70	Joback Method
dvisc	0.0020794	Pa×s	332.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354636&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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