4-Isopropylphenoxyacetic acid

Inchi: InChI=1S/C11H14O3/c1-8(2)9-3-5-10(6-4-9)14-7-11(12)13/h3-6,8H,7H2,1-2H3,(H,12,13)
InchiKey: FPVCSFOUVDLTDG-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CC(C)c1ccc(OCC(=O)O)cc1
Mol. weight [g/mol]: 194.23
CAS: 1643-16-9

Physical Properties

Property code	Value	Unit	Source
gf	-228.66	kJ/mol	Joback Method
hf	-447.62	kJ/mol	Joback Method
hfus	21.25	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.273		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	650.77	K	Joback Method
tc	851.23	K	Joback Method
tf	370.65	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.51	J/mol×K	650.77	Joback Method
cpg	452.28	J/mol×K	817.82	Joback Method
cpg	443.04	J/mol×K	784.41	Joback Method
cpg	433.16	J/mol×K	751.00	Joback Method
cpg	422.62	J/mol×K	717.59	Joback Method
cpg	411.41	J/mol×K	684.18	Joback Method
cpg	460.89	J/mol×K	851.23	Joback Method
dvisc	0.0000526	Pa×s	650.77	Joback Method
dvisc	0.0000793	Pa×s	604.08	Joback Method

dvisc	0.0001280	Pa×s	557.40	Joback Method
dvisc	0.0002256	Pa×s	510.71	Joback Method
dvisc	0.0004455	Pa×s	464.02	Joback Method
dvisc	0.0010245	Pa×s	417.34	Joback Method
dvisc	0.0029058	Pa×s	370.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1643169&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume