Propanal, 2-methyl-2-(4-isopropylphenyl)

Inchi: InChI=1S/C13H18O/c1-10(2)11-5-7-12(8-6-11)13(3,4)9-14/h5-10H,1-4H3
InchiKey: HGECJFVPNUYRJZ-UHFFFAOYSA-N
Formula: C13H18O
SMILES: CC(C)c1ccc(C(C)(C)C=O)cc1
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
gf	62.24	kJ/mol	Joback Method
hf	-186.20	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	52.51	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.287		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1444.00		NIST Webbook
rinpol	1444.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1954.00		NIST Webbook
tb	573.49	K	Joback Method
tc	791.49	K	Joback Method
tf	304.63	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.75	J/mol×K	573.49	Joback Method
cpg	437.67	J/mol×K	609.82	Joback Method
cpg	453.47	J/mol×K	646.16	Joback Method
cpg	468.21	J/mol×K	682.49	Joback Method
cpg	481.95	J/mol×K	718.82	Joback Method
cpg	494.76	J/mol×K	755.15	Joback Method

cpg	506.68	J/mol×K	791.49	Joback Method
dvisc	0.0040558	Pa×s	304.63	Joback Method
dvisc	0.0017567	Pa×s	349.44	Joback Method
dvisc	0.0009203	Pa×s	394.25	Joback Method
dvisc	0.0005501	Pa×s	439.06	Joback Method
dvisc	0.0003617	Pa×s	483.87	Joback Method
dvisc	0.0002554	Pa×s	528.68	Joback Method
dvisc	0.0001904	Pa×s	573.49	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=R410161&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume