2-((2-Ethylbutoxy)carbonyl)benzoic acid

Inchi: InChI=1S/C14H18O4/c1-3-10(4-2)9-18-14(17)12-8-6-5-7-11(12)13(15)16/h5-8,10H,3-4,9
InchiKey: XSLWVQWUWZGQNV-UHFFFAOYSA-N
Formula: C14H18O4
SMILES: CCC(CC)COC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 250.29
CAS: 91401-46-6

Physical Properties

Property code	Value	Unit	Source
gf	-332.32	kJ/mol	Joback Method
hf	-622.12	kJ/mol	Joback Method
hfus	30.62	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.978		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1977.00		NIST Webbook
tb	773.28	K	Joback Method
tc	974.61	K	Joback Method
tf	454.39	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.11	J/mol×K	773.28	Joback Method
cpg	621.77	J/mol×K	941.05	Joback Method
cpg	612.79	J/mol×K	907.50	Joback Method
cpg	603.06	J/mol×K	873.94	Joback Method
cpg	592.54	J/mol×K	840.39	Joback Method
cpg	581.23	J/mol×K	806.83	Joback Method
cpg	630.02	J/mol×K	974.61	Joback Method
dvisc	0.0000274	Pa×s	773.28	Joback Method

dvisc	0.0000401	Pa×s	720.13	Joback Method
dvisc	0.0000623	Pa×s	666.98	Joback Method
dvisc	0.0001045	Pa×s	613.84	Joback Method
dvisc	0.0001933	Pa×s	560.69	Joback Method
dvisc	0.0004068	Pa×s	507.54	Joback Method
dvisc	0.0010185	Pa×s	454.39	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=C91401466&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

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