

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.11	J/molxK	773.28	Joback Method
cpg	581.23	J/molxK	806.83	Joback Method
cpg	592.54	J/molxK	840.39	Joback Method
cpg	603.06	J/molxK	873.94	Joback Method
cpg	612.79	J/molxK	907.50	Joback Method
cpg	621.77	J/molxK	941.05	Joback Method
cpg	630.02	J/molxK	974.61	Joback Method
dvisc	0.0010185	Paxs	454.39	Joback Method

dvisc	0.0004068	Paxs	507.54	Joback Method
dvisc	0.0001933	Paxs	560.69	Joback Method
dvisc	0.0001045	Paxs	613.84	Joback Method
dvisc	0.0000623	Paxs	666.98	Joback Method
dvisc	0.0000401	Paxs	720.13	Joback Method
dvisc	0.0000274	Paxs	773.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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