2-(Allyloxycarbonyl)benzoic acid

Inchi:	InChI=1S/C11H10O4/c1-2-7-15-11(14)9-6-4-3-5-8(9)10(12)13/h2-6H,1,7H2,(H,12,13)
InchiKey:	UIYHUUARNKRKGV-UHFFFAOYSA-N
Formula:	C11H10O4
SMILES:	C=CCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]:	206.19
CAS:	3882-14-2

Physical Properties

Property code	Value	Unit	Source
gf	-267.30	kJ/mol	Joback Method
hf	-429.49	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	74.93	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.728		Crippen Method
mcvol	152.670	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	1723.00		NIST Webbook
tb	701.76	K	Joback Method
tc	908.73	K	Joback Method
tf	433.82	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.16	J/mol×K	701.76	Joback Method
cpg	397.92	J/mol×K	736.25	Joback Method
cpg	407.02	J/mol×K	770.75	Joback Method
cpg	415.47	J/mol×K	805.24	Joback Method
cpg	423.29	J/mol×K	839.74	Joback Method
cpg	430.51	J/mol×K	874.23	Joback Method
cpg	437.14	J/mol×K	908.73	Joback Method
dvisc	0.0012456	Pa×s	433.82	Joback Method

dvisc	0.0005745	Pa×s	478.48	Joback Method
dvisc	0.0003024	Pa×s	523.13	Joback Method
dvisc	0.0001761	Pa×s	567.79	Joback Method
dvisc	0.0001109	Pa×s	612.45	Joback Method
dvisc	0.0000744	Pa×s	657.10	Joback Method
dvisc	0.0000525	Pa×s	701.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3882142&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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