Anthranilic acid, isopropyl ester

Other names:	Anthranilic acid, isopropyl ester
	Isopropyl anthranilate
	Isopropyl 2-aminobenzoate
Inchi:	InChI=1S/C10H13NO2/c1-7(2)13-10(12)8-5-3-4-6-9(8)11/h3-7H,11H2,1-2H3
InchiKey:	XKOZHFJYXAQZJX-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CC(C)OC(=O)c1ccccc1N
Mol. weight [g/mol]:	179.22

Physical Properties

Property code	Value	Unit	Source
hf	-350.54	kJ/mol	Cheméo Relay (1.0)
hfus	19.77	kJ/mol	Joback Method
ie	7.96	eV	Cheméo Relay (1.0)
log10ws	-2.84		Cheméo Relay (1.0)
logp	1.834		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	536.61	K	Cheméo Relay (1.0)
tf	290.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.55	J/mol×K	608.24	Joback Method
cpg	370.93	J/mol×K	646.05	Joback Method
cpg	383.46	J/mol×K	683.85	Joback Method
cpg	395.16	J/mol×K	721.66	Joback Method
cpg	406.06	J/mol×K	759.47	Joback Method
cpg	416.18	J/mol×K	797.28	Joback Method
cpg	425.52	J/mol×K	835.08	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18189021&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point