BUTYL 2-PYRIDINECARBOXYLATE

Other names:	butyl picolinate
	butyl pyridine-2-carboxylate
Inchi:	InChI=1S/C10H13NO2/c1-2-3-8-13-10(12)9-6-4-5-7-11-9/h4-7H,2-3,8H2,1H3
InchiKey:	HZUPDAXALKWCGX-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCCCOC(=O)c1ccccn1
Mol. weight [g/mol]:	179.22

Physical Properties

Property code	Value	Unit	Source
af	0.5877		Cheméo Relay (1.0)
hf	-283.33	kJ/mol	Cheméo Relay (1.0)
hvap	66.50	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-2.28		Cheméo Relay (1.0)
logp	2.038		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2720.22	kPa	Cheméo Relay (1.0, beta)
tb	531.73	K	Cheméo Relay (1.0)
tc	733.86	K	Cheméo Relay (1.0)
tf	233.19	K	Cheméo Relay (1.0)
vc	0.544	m3/kmol	Cheméo Relay (1.0)

Sources

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=C5340885&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume