Methyl pyrazine-2-carboxylate

Inchi: InChI=1S/C6H6N2O2/c1-10-6(9)5-4-7-2-3-8-5/h2-4H,1H3
InchiKey: TWIIRMSFZNYMQE-UHFFFAOYSA-N
Formula: C6H6N2O2
SMILES: COC(=O)c1cnccn1
Mol. weight [g/mol]: 138.13

Physical Properties

Property code	Value	Unit	Source
hvap	64.26	kJ/mol	Cheméo Relay (1.0)
ie	9.52	eV	Cheméo Relay (1.0)
log10ws	-0.48		Cheméo Relay (1.0)
logp	0.263		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
tb	490.21	K	Cheméo Relay (1.0)
tf	331.13	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C6164790
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):

Legend

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point