5-ETHYL-2-FURALDEHYDE

Other names: 2-Furancarboxaldehyde, 5-ethyl-
5-Ethylfurfural
Furan-2-carboxaldehyde, 5-ethyl
Inchi: InChI=1S/C7H8O2/c1-2-6-3-4-7(5-8)9-6/h3-5H,2H2,1H3
InchiKey: XADGZBXFWQHBDB-UHFFFAOYSA-N
Formula: C7H8O2
SMILES: CCc1ccc(C=O)o1
Mol. weight [g/mol]: 124.14

Physical Properties

Property code	Value	Unit	Source
hf	-238.91	kJ/mol	Cheméo Relay (1.0)
hvap	54.83	kJ/mol	Cheméo Relay (1.0)
logp	1.655		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1641.00		NIST Webbook
tb	455.86	K	Cheméo Relay (1.0)
tf	243.47	K	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=C23074104&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point