2-HEXYLFURAN

Other names: 2-Hexylfuran
2-n-Hexylfuran
Inchi: InChI=1S/C10H16O/c1-2-3-4-5-7-10-8-6-9-11-10/h6,8-9H,2-5,7H2,1H3
InchiKey: XBLCAKKYMZVLPU-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CCCCCCc1ccco1
Mol. weight [g/mol]: 152.24

Physical Properties

Property code	Value	Unit	Source
af	0.4892		Cheméo Relay (1.0)
hf	-174.50	kJ/mol	Cheméo Relay (1.0)
hvap	52.52	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-3.31		Cheméo Relay (1.0)
logp	3.402		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2630.58	kPa	Cheméo Relay (1.0, beta)
rinpol	1096.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1079.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1312.00		NIST Webbook

ripol	1312.00		NIST Webbook
ripol	1316.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1332.00		NIST Webbook
tb	461.02	K	Cheméo Relay (1.0)
tc	647.36	K	Cheméo Relay (1.0)
tf	218.11	K	Cheméo Relay (1.0)
vc	0.547	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3777706&Units=SI
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

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume