1-HEPTANONE, 1-(2-FURANYL)-

Other names: 2-Heptanoylfuran
Furan, 2-heptanoyl
Inchi: InChI=1S/C11H16O2/c1-2-3-4-5-7-10(12)11-8-6-9-13-11/h6,8-9H,2-5,7H2,1H3
InchiKey: BTNRWSUWLFMXEL-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CCCCCCC(=O)c1ccco1
Mol. weight [g/mol]: 180.25

Physical Properties

Property code	Value	Unit	Source
af	0.5980		Cheméo Relay (1.0)
hf	-317.97	kJ/mol	Cheméo Relay (1.0)
hvap	65.37	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-3.66		Cheméo Relay (1.0)
logp	3.433		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2369.25	kPa	Cheméo Relay (1.0, beta)
ripol	1956.00		NIST Webbook
ripol	1956.00		NIST Webbook
tb	519.53	K	Cheméo Relay (1.0)
tc	713.40	K	Cheméo Relay (1.0)
tf	291.05	K	Cheméo Relay (1.0)
vc	0.597	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5466400&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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