2-HEPTYLFURAN

Other names: Furan, 2-heptyl-
Inchi: InChI=1S/C11H18O/c1-2-3-4-5-6-8-11-9-7-10-12-11/h7,9-10H,2-6,8H2,1H3
InchiKey: BHTUFJXTYNLISA-UHFFFAOYSA-N
Formula: C11H18O
SMILES: CCCCCCCc1ccco1
Mol. weight [g/mol]: 166.26
CAS: 3777-71-7

Physical Properties

Property code	Value	Unit	Source
af	0.5367		Cheméo Relay (1.0)
hf	-195.32	kJ/mol	Cheméo Relay (1.0)
hvap	57.33	kJ/mol	Cheméo Relay (1.0)
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-3.88		Cheméo Relay (1.0)
logp	3.793		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2448.86	kPa	Cheméo Relay (1.0, beta)
rinpol	1186.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1188.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1429.00		NIST Webbook

ripol	1417.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1448.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1416.00		NIST Webbook
tb	480.74	K	Cheméo Relay (1.0)
tc	666.52	K	Cheméo Relay (1.0)
tf	232.53	K	Cheméo Relay (1.0)
vc	0.605	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42324e+01
Coeff. B	-3.91069e+03
Coeff. C	-7.08790e+01
Temperature range (K), min.	351.32
Temperature range (K), max.	509.25

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3777717&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):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor 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