2-n-Heptylfuran

Other names:	2-Heptylfuran
	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
log10ws	-8.10		Crippen Method
logp	3.792		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
rinpol	1195.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1184.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1448.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1429.00		NIST Webbook

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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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