FURFURYL OCTANOATE

Other names: Furfuryl octanoate
Inchi: InChI=1S/C13H20O3/c1-2-3-4-5-6-9-13(14)16-11-12-8-7-10-15-12/h7-8,10H,2-6,9,11H2,
InchiKey: JNIWCVWKECYDSV-UHFFFAOYSA-N
Formula: C13H20O3
SMILES: CCCCCCCC(=O)OCc1ccco1
Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
hf	-534.91	kJ/mol	Cheméo Relay (1.0)
hvap	71.01	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
log10ws	-3.76		Cheméo Relay (1.0)
logp	3.683		Crippen Method
mcvol	187.880	ml/mol	McGowan Method
pc	2043.96	kPa	Cheméo Relay (1.0, beta)
rinpol	1543.00		NIST Webbook
tb	548.15	K	Cheméo Relay (1.0)
tc	735.69	K	Cheméo Relay (1.0)
tf	259.39	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39252034&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

Legend

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point