METHYL 7-(2-FUROYL)HEPTANOATE

Other names: Octanoic acid, 8-oxo-8-(2-furyl), ethyl ester
Inchi: InChI=1S/C13H18O4/c1-16-13(15)9-5-3-2-4-7-11(14)12-8-6-10-17-12/h6,8,10H,2-5,7,9H
InchiKey: YEJWQYJOGFNXRR-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: COC(=O)CCCCCCC(=O)c1ccco1
Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
hf	-655.97	kJ/mol	Cheméo Relay (1.0)
hvap	86.75	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-3.18		Cheméo Relay (1.0)
logp	2.976		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2070.97	kPa	Cheméo Relay (1.0, beta)
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tb	581.48	K	Cheméo Relay (1.0)
tc	767.17	K	Cheméo Relay (1.0)
tf	317.42	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38199472&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

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