PHENETHYL 2-FUROATE

Other names:	2-Furoic acid, phenethyl ester
	AI3-36016
	Phenethyl 2-furoate
	2-Furanecarboxylic acid, 2-phenylethyl ester
	2-Phenylethyl 2-furoate
Inchi:	InChI=1S/C13H12O3/c14-13(12-7-4-9-15-12)16-10-8-11-5-2-1-3-6-11/h1-7,9H,8,10H2
InchiKey:	QKPSYARWSBJEDY-UHFFFAOYSA-N
Formula:	C13H12O3
SMILES:	O=C(OCCc1ccccc1)c1ccco1
Mol. weight [g/mol]:	216.24

Physical Properties

Property code	Value	Unit	Source
hf	-287.36	kJ/mol	Cheméo Relay (1.0)
hvap	84.47	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	-3.48		Cheméo Relay (1.0)
logp	2.679		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
pc	2651.85	kPa	Cheméo Relay (1.0, beta)
rinpol	1760.00		NIST Webbook
tb	591.77	K	Cheméo Relay (1.0)
tf	271.26	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7149328&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
tf:	Normal melting (fusion) point