n-Amyl furylpropionate

Other names: Amyl furfuryl propionate
Inchi: InChI=1S/C12H18O3/c1-2-3-4-9-15-12(13)8-7-11-6-5-10-14-11/h5-6,10H,2-4,7-9H2,1H3
InchiKey: MRNLJBGPIOBGFP-UHFFFAOYSA-N
Formula: C12H18O3
SMILES: CCCCCOC(=O)CCc1ccco1
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
hf	-525.10	kJ/mol	Cheméo Relay (1.0)
hvap	67.69	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.74		Cheméo Relay (1.0)
logp	2.946		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2252.83	kPa	Cheméo Relay (1.0, beta)
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
ripol	1947.00		NIST Webbook
tb	536.41	K	Cheméo Relay (1.0)
tc	721.32	K	Cheméo Relay (1.0)
tf	240.18	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U284966&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point