2-((Pent-4-enyloxy)carbonyl)benzoic acid

Inchi: InChI=1S/C13H14O4/c1-2-3-6-9-17-13(16)11-8-5-4-7-10(11)12(14)15/h2,4-5,7-8H,1,3,6,
InchiKey: HYCQCFCIEMXEMJ-UHFFFAOYSA-N
Formula: C13H14O4
SMILES: C=CCCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 234.25
CAS: 190184-82-8

Physical Properties

Property code	Value	Unit	Source
gf	-250.46	kJ/mol	Joback Method
hf	-470.77	kJ/mol	Joback Method
hfus	30.27	kJ/mol	Joback Method
hvap	79.38	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.508		Crippen Method
mcvol	180.850	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	747.52	K	Joback Method
tc	950.11	K	Joback Method
tf	456.36	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.32	J/mol×K	747.52	Joback Method
cpg	537.76	J/mol×K	916.34	Joback Method
cpg	529.65	J/mol×K	882.58	Joback Method
cpg	520.87	J/mol×K	848.81	Joback Method
cpg	511.41	J/mol×K	815.05	Joback Method
cpg	501.23	J/mol×K	781.28	Joback Method
cpg	545.23	J/mol×K	950.11	Joback Method

dvisc	0.0000377	Pa×s	747.52	Joback Method
dvisc	0.0000536	Pa×s	698.99	Joback Method
dvisc	0.0000802	Pa×s	650.47	Joback Method
dvisc	0.0001282	Pa×s	601.94	Joback Method
dvisc	0.0002226	Pa×s	553.41	Joback Method
dvisc	0.0004296	Pa×s	504.89	Joback Method
dvisc	0.0009534	Pa×s	456.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C190184828&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume