1,2-Benzenedicarboxylic acid, monopentyl ester

Inchi: InChI=1S/C13H16O4/c1-2-3-6-9-17-13(16)11-8-5-4-7-10(11)12(14)15/h4-5,7-8H,2-3,6,9H

InchiKey: FPGPRAKRYDSZAW-UHFFFAOYSA-N

Formula: C13H16O4

SMILES: CCCCCOC(=O)c1ccccc1C(=O)O

Mol. weight [g/mol]: 236.27

Physical Properties

Property code	Value	Unit	Source
af	0.9180		Cheméo Relay (1.0)
hf	-704.65	kJ/mol	Cheméo Relay (1.0)
hfus	31.55	kJ/mol	Joback Method
hvap	99.59	kJ/mol	Cheméo Relay (1.0)
ie	9.36	eV	Cheméo Relay (1.0)
log10ws	-3.47		Cheméo Relay (1.0)
logp	2.732		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	592.64	K	Cheméo Relay (1.0)
tc	824.76	K	Cheméo Relay (1.0)
tf	347.82	K	Cheméo Relay (1.0)
vc	0.676	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.99	J/mol×K	750.84	Joback Method
cpg	573.14	J/mol×K	950.74	Joback Method
cpg	565.21	J/mol×K	917.42	Joback Method
cpg	556.60	J/mol×K	884.10	Joback Method
cpg	547.29	J/mol×K	850.79	Joback Method
cpg	537.26	J/mol×K	817.47	Joback Method
cpg	526.50	J/mol×K	784.16	Joback Method

dvisc	0.0001223	Pa×s	604.48	Joback Method
dvisc	0.0000353	Pa×s	750.84	Joback Method
dvisc	0.0000505	Pa×s	702.05	Joback Method
dvisc	0.0000760	Pa×s	653.27	Joback Method
dvisc	0.0009364	Pa×s	458.12	Joback Method
dvisc	0.0002140	Pa×s	555.69	Joback Method
dvisc	0.0004170	Pa×s	506.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24539568&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
vc:	Critical Volume