Pent-2-en-1-yl benzoate

Inchi: InChI=1S/C12H14O2/c1-2-3-7-10-14-12(13)11-8-5-4-6-9-11/h3-9H,2,10H2,1H3/b7-3+
InchiKey: CSDCIXOZTUVBQA-XVNBXDOJSA-N
Formula: C12H14O2
SMILES: CCC=CCOC(=O)c1ccccc1
Mol. weight [g/mol]: 190.24
CAS: 65416-27-5

Physical Properties

Property code	Value	Unit	Source
gf	8.87	kJ/mol	Joback Method
hf	-182.06	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	53.70	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.810		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1492.00		NIST Webbook
tb	581.09	K	Joback Method
tc	796.06	K	Joback Method
tf	318.50	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.36	J/mol×K	581.09	Joback Method
cpg	389.03	J/mol×K	616.92	Joback Method
cpg	402.78	J/mol×K	652.75	Joback Method
cpg	415.66	J/mol×K	688.57	Joback Method
cpg	427.72	J/mol×K	724.40	Joback Method
cpg	438.98	J/mol×K	760.23	Joback Method
cpg	449.48	J/mol×K	796.06	Joback Method
dvisc	0.0020709	Pa×s	318.50	Joback Method

dvisc	0.0010390	Pa×s	362.26	Joback Method
dvisc	0.0006049	Pa×s	406.03	Joback Method
dvisc	0.0003912	Pa×s	449.80	Joback Method
dvisc	0.0002734	Pa×s	493.56	Joback Method
dvisc	0.0002025	Pa×s	537.33	Joback Method
dvisc	0.0001569	Pa×s	581.09	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=C65416275&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