

4-Pentenyl benzoate

Inchi:	InChI=1S/C12H14O2/c1-2-3-7-10-14-12(13)11-8-5-4-6-9-11/h2,4-6,8-9H,1,3,7,10H2
InchiKey:	MFUGAJWSACDNNH-UHFFFAOYSA-N
Formula:	C12H14O2
SMILES:	C=CCCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	190.24

Physical Properties

Property code	Value	Unit	Source
gf	16.49	kJ/mol	Joback Method
hf	-173.85	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	53.07	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.810		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1442.00		NIST Webbook
ripol	1986.00		NIST Webbook
ripol	2016.00		NIST Webbook
ripol	2016.00		NIST Webbook
ripol	2008.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	1986.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2028.00		NIST Webbook
ripol	2009.00		NIST Webbook

ripol	2012.00		NIST Webbook
tb	573.61	K	Joback Method
tc	783.80	K	Joback Method
tf	321.82	K	Joback Method
vc	0.605	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.80	J/molxK	573.61	Joback Method
cpg	388.35	J/molxK	608.64	Joback Method
cpg	402.04	J/molxK	643.67	Joback Method
cpg	414.90	J/molxK	678.70	Joback Method
cpg	426.96	J/molxK	713.74	Joback Method
cpg	438.23	J/molxK	748.77	Joback Method
cpg	448.76	J/molxK	783.80	Joback Method
dvisc	0.0021457	Paxs	321.82	Joback Method
dvisc	0.0011349	Paxs	363.79	Joback Method
dvisc	0.0006848	Paxs	405.75	Joback Method
dvisc	0.0004542	Paxs	447.72	Joback Method
dvisc	0.0003233	Paxs	489.68	Joback Method
dvisc	0.0002428	Paxs	531.64	Joback Method
dvisc	0.0001901	Paxs	573.61	Joback Method

Sources

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=R30929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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