

Benzoic acid, neopentyl ester

Inchi:	InChI=1S/C12H16O2/c1-12(2,3)9-14-11(13)10-7-5-4-6-8-10/h4-8H,9H2,1-3H3
InchiKey:	ZBPDCWGVJKTGND-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CC(C)(C)COC(=O)c1ccccc1
Mol. weight [g/mol]:	192.25

Physical Properties

Property code	Value	Unit	Source
gf	-68.51	kJ/mol	Joback Method
hf	-308.03	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	52.44	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.889		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1382.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1382.00		NIST Webbook
tb	573.70	K	Joback Method
tc	792.31	K	Joback Method
tf	326.00	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.32	J/molxK	573.70	Joback Method
cpg	413.41	J/molxK	610.13	Joback Method
cpg	428.45	J/molxK	646.57	Joback Method
cpg	442.47	J/molxK	683.00	Joback Method
cpg	455.52	J/molxK	719.44	Joback Method
cpg	467.66	J/molxK	755.87	Joback Method
cpg	478.93	J/molxK	792.31	Joback Method

dvisc	0.0026378	Paxs	326.00	Joback Method
dvisc	0.0012864	Paxs	367.28	Joback Method
dvisc	0.0007254	Paxs	408.57	Joback Method
dvisc	0.0004544	Paxs	449.85	Joback Method
dvisc	0.0003079	Paxs	491.13	Joback Method
dvisc	0.0002216	Paxs	532.42	Joback Method
dvisc	0.0001672	Paxs	573.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U357793&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

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