

Benzoic acid, 4-(neopentyl)oxy-, methyl ester

Inchi:	InChI=1S/C13H18O3/c1-13(2,3)9-16-11-7-5-10(6-8-11)12(14)15-4/h5-8H,9H2,1-4H3
InchiKey:	UOCIVMZNSMYJHR-UHFFFAOYSA-N
Formula:	C13H18O3
SMILES:	<chem>COC(=O)c1ccc(OCC(C)(C)C)cc1</chem>
Mol. weight [g/mol]:	222.28

Physical Properties

Property code	Value	Unit	Source
gf	-174.72	kJ/mol	Joback Method
hf	-472.36	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	57.74	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.898		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinqol	1644.00		NIST Webbook
tb	623.98	K	Joback Method
tc	837.28	K	Joback Method
tf	372.02	K	Joback Method
vc	0.686	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.53	J/molxK	623.98	Joback Method
cpg	488.51	J/molxK	659.53	Joback Method
cpg	503.52	J/molxK	695.08	Joback Method
cpg	517.57	J/molxK	730.63	Joback Method
cpg	530.70	J/molxK	766.18	Joback Method
cpg	542.93	J/molxK	801.73	Joback Method
cpg	554.30	J/molxK	837.28	Joback Method
dvisc	0.0013196	Paxs	372.02	Joback Method
dvisc	0.0007150	Paxs	414.01	Joback Method

dvisc	0.0004337	Paxs	456.01	Joback Method
dvisc	0.0002862	Paxs	498.00	Joback Method
dvisc	0.0002015	Paxs	539.99	Joback Method
dvisc	0.0001492	Paxs	581.99	Joback Method
dvisc	0.0001151	Paxs	623.98	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=U375326&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
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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