

Benzoic acid, 3-methyl-, 2-methylpentyl ester

Inchi:	InChI=1S/C14H20O2/c1-4-6-12(3)10-16-14(15)13-8-5-7-11(2)9-13/h5,7-9,12H,4,6,10H2,
InchiKey:	OZKOMPPHFFQKGN-UHFFFAOYSA-N
Formula:	C14H20O2
SMILES:	CCCC(C)COC(=O)c1cccc(C)c1
Mol. weight [g/mol]:	220.31

Physical Properties

Property code	Value	Unit	Source
gf	-66.58	kJ/mol	Joback Method
hf	-357.31	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	58.46	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.588		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1667.00		NIST Webbook
tb	627.23	K	Joback Method
tc	832.03	K	Joback Method
tf	343.64	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.28	J/molxK	627.23	Joback Method
cpg	510.76	J/molxK	661.36	Joback Method
cpg	526.32	J/molxK	695.50	Joback Method
cpg	540.99	J/molxK	729.63	Joback Method
cpg	554.78	J/molxK	763.76	Joback Method
cpg	567.73	J/molxK	797.90	Joback Method
cpg	579.84	J/molxK	832.03	Joback Method
dvisc	0.0019801	Paxs	343.64	Joback Method
dvisc	0.0009738	Paxs	390.90	Joback Method

dvisc	0.0005582	Paxs	438.17	Joback Method
dvisc	0.0003565	Paxs	485.44	Joback Method
dvisc	0.0002466	Paxs	532.70	Joback Method
dvisc	0.0001811	Paxs	579.97	Joback Method
dvisc	0.0001394	Paxs	627.23	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=U355708&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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