

Benzoic acid, 4-(1-methylpropyl)oxy-, 1-methylpropyl ester

Inchi:	InChI=1S/C15H22O3/c1-5-11(3)17-14-9-7-13(8-10-14)15(16)18-12(4)6-2/h7-12H,5-6H2,
InchiKey:	CADVQIQXKHEZIB-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	CCC(C)OC(=O)c1ccc(OC(C)CC)cc1
Mol. weight [g/mol]:	250.33

Physical Properties

Property code	Value	Unit	Source
gf	-165.60	kJ/mol	Joback Method
hf	-515.45	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.819		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1796.00		NIST Webbook
tb	672.09	K	Joback Method
tc	875.92	K	Joback Method
tf	362.14	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.95	J/molxK	672.09	Joback Method
cpg	649.82	J/molxK	841.94	Joback Method
cpg	636.74	J/molxK	807.97	Joback Method
cpg	622.73	J/molxK	774.00	Joback Method
cpg	607.76	J/molxK	740.03	Joback Method
cpg	591.84	J/molxK	706.06	Joback Method
cpg	661.98	J/molxK	875.92	Joback Method
dvisc	0.0000909	Paxs	672.09	Joback Method
dvisc	0.0001204	Paxs	620.43	Joback Method

dvisc	0.0001679	Paxs	568.77	Joback Method
dvisc	0.0002501	Paxs	517.12	Joback Method
dvisc	0.0004072	Paxs	465.46	Joback Method
dvisc	0.0007488	Paxs	413.80	Joback Method
dvisc	0.0016383	Paxs	362.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375442&Units=SI
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

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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