

Cinnarizine M (hydroxy-methoxy-benzophenone), isomer 2,

InChI: **acetylated** InChI=1S/C16H14O4/c1-11(17)20-14-9-8-13(10-15(14)19-2)16(18)12-6-4-3-5-7-12/h3-10

InChIKey: WFCCWTDFFHGWRCG-UHFFFAOYSA-N

Formula: C16H14O4

SMILES: COc1cc(C(=O)c2ccccc2)ccc1OC(C)=O

Mol. weight [g/mol]: 270.28

Physical Properties

Property code	Value	Unit	Source
gf	-178.44	kJ/mol	Joback Method
hf	-413.05	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	75.40	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	2.851		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	781.38	K	Joback Method
tc	1018.00	K	Joback Method
tf	492.28	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.14	J/molxK	781.38	Joback Method
cpg	612.41	J/molxK	978.56	Joback Method
cpg	603.68	J/molxK	939.12	Joback Method
cpg	593.81	J/molxK	899.69	Joback Method
cpg	582.77	J/molxK	860.25	Joback Method
cpg	570.55	J/molxK	820.82	Joback Method
cpg	620.03	J/molxK	1018.00	Joback Method

dvisc	0.0000953	Paxs	781.38	Joback Method
dvisc	0.0001178	Paxs	733.20	Joback Method
dvisc	0.0001500	Paxs	685.01	Joback Method
dvisc	0.0001981	Paxs	636.83	Joback Method
dvisc	0.0002738	Paxs	588.65	Joback Method
dvisc	0.0004009	Paxs	540.46	Joback Method
dvisc	0.0006325	Paxs	492.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R536213&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
mvol:	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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