

Cinnarizine M (hydroxy-benzophenone), isomer 1, acetylated

Inchi: InChI=1S/C15H12O3/c1-11(16)18-14-10-6-5-9-13(14)15(17)12-7-3-2-4-8-12/h2-10H,1H3
InchiKey: ZTTANZQQBIQFEG-UHFFFAOYSA-N
Formula: C15H12O3
SMILES: CC(=O)Oc1ccccc1C(=O)c1ccccc1
Mol. weight [g/mol]: 240.25

Physical Properties

Property code	Value	Unit	Source
gf	-72.23	kJ/mol	Joback Method
hf	-248.72	kJ/mol	Joback Method
hfus	26.68	kJ/mol	Joback Method
hvap	70.10	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.843		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	731.10	K	Joback Method
tc	975.09	K	Joback Method
tf	446.26	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.02	J/mol×K	731.10	Joback Method
cpg	536.90	J/mol×K	934.42	Joback Method
cpg	527.71	J/mol×K	893.76	Joback Method
cpg	517.48	J/mol×K	853.09	Joback Method
cpg	506.15	J/mol×K	812.43	Joback Method
cpg	493.68	J/mol×K	771.76	Joback Method
cpg	545.09	J/mol×K	975.09	Joback Method
dvisc	0.0001379	Pa×s	731.10	Joback Method
dvisc	0.0001724	Pa×s	683.63	Joback Method
dvisc	0.0002229	Pa×s	636.15	Joback Method

dvisc	0.0003004	Pa×s	588.68	Joback Method
dvisc	0.0004265	Pa×s	541.21	Joback Method
dvisc	0.0006479	Pa×s	493.73	Joback Method
dvisc	0.0010757	Pa×s	446.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R536184&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/93-616-5/Cinnarizine-M-hydroxy-benzophenone-isomer-1-acetylated.pdf>

Generated by Cheméo on 2025-12-06 00:34:16.5062699 +0000 UTC m=+4729454.036310554.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.