

3-(Hydroxyphenylmethyl)-3,4-dimethyl-1-phenylpropan-1-one

Inchi:	InChI=1S/C20H24O2/c1-15(2)20(3,19(22)17-12-8-5-9-13-17)18(21)14-16-10-6-4-7-11-16
InchiKey:	HMLHBLHHYRCPRN-UHFFFAOYSA-N
Formula:	C20H24O2
SMILES:	CC(C)C(C)(C(=O)Cc1ccccc1)C(O)c1ccccc1
Mol. weight [g/mol]:	296.40
CAS:	97234-51-0

Physical Properties

Property code	Value	Unit	Source
gf	74.56	kJ/mol	Joback Method
hf	-267.19	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	86.02	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.194		Crippen Method
mcvol	252.580	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
tb	852.30	K	Joback Method
tc	1076.83	K	Joback Method
tf	451.17	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.30	J/molxK	852.30	Joback Method
cpg	786.96	J/molxK	889.72	Joback Method
cpg	800.55	J/molxK	927.14	Joback Method
cpg	813.17	J/molxK	964.56	Joback Method
cpg	824.93	J/molxK	1001.98	Joback Method
cpg	835.96	J/molxK	1039.40	Joback Method
cpg	846.34	J/molxK	1076.83	Joback Method
dvisc	0.0012064	Paxs	451.17	Joback Method
dvisc	0.0003290	Paxs	518.02	Joback Method

dvisc	0.0001207	Paxs	584.88	Joback Method
dvisc	0.0000544	Paxs	651.74	Joback Method
dvisc	0.0000285	Paxs	718.59	Joback Method
dvisc	0.0000166	Paxs	785.44	Joback Method
dvisc	0.0000106	Paxs	852.30	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=C97234510&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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