

3-HYDROXY-4-METHYLBENZOIC ACID

Other names:	Benzoic acid, 3-hydroxy-4-methyl- 3,4-Cresotic acid 3-hydroxy-p-toluic acid
Inchi:	InChI=1S/C8H8O3/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4,9H,1H3,(H,10,11)
InchiKey:	ZQLCWPXBHUALQC-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	Cc1ccc(C(=O)O)cc1O
Mol. weight [g/mol]:	152.15

Physical Properties

Property code	Value	Unit	Source
hf	-502.81	kJ/mol	Cheméo Relay (1.0)
hfus	21.60	kJ/mol	Joback Method
hvap	108.93	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	Cheméo Relay (1.0)
log10ws	-1.40		Cheméo Relay (1.0)
logp	1.399		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
tb	551.51	K	Cheméo Relay (1.0)
tc	820.10	K	Cheméo Relay (1.0)
tf	475.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.61	J/mol×K	640.77	Joback Method
cpg	318.35	J/mol×K	858.15	Joback Method
cpg	312.29	J/mol×K	821.92	Joback Method
cpg	305.95	J/mol×K	785.69	Joback Method
cpg	299.28	J/mol×K	749.46	Joback Method
cpg	292.21	J/mol×K	713.23	Joback Method
cpg	284.67	J/mol×K	677.00	Joback Method
dvisc	0.0000568	Pa×s	541.05	Joback Method
dvisc	0.0000116	Pa×s	640.77	Joback Method

dvisc	0.0000186	Pa×s	607.53	Joback Method
dvisc	0.0000314	Pa×s	574.29	Joback Method
dvisc	0.0005703	Pa×s	441.33	Joback Method
dvisc	0.0001108	Pa×s	507.81	Joback Method
dvisc	0.0002373	Pa×s	474.57	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C586301&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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