

1,3-dimethyl-isochroman, 1a', 3e

Inchi:	InChI=1S/C11H14O/c1-8-7-10-5-3-4-6-11(10)9(2)12-8/h3-6,8-9H,7H2,1-2H3/t8-,9-/m1/s1
InchiKey:	AIODYCJUHTYCEB-RKDXNWHRSA-N
Formula:	C11H14O
SMILES:	CC1Cc2ccccc2C(C)O1
Mol. weight [g/mol]:	162.23

Physical Properties

Property code	Value	Unit	Source
gf	99.34	kJ/mol	Joback Method
hf	-131.01	kJ/mol	Joback Method
hfus	22.98	kJ/mol	Joback Method
hvap	47.30	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.709		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1256.60		NIST Webbook
rinpol	1256.60		NIST Webbook
ripol	1728.80		NIST Webbook
tb	516.03	K	Joback Method
tc	742.26	K	Joback Method
tf	289.42	K	Joback Method
vc	0.512	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.39	J/molxK	516.03	Joback Method
cpg	335.94	J/molxK	553.74	Joback Method
cpg	352.37	J/molxK	591.44	Joback Method
cpg	367.75	J/molxK	629.15	Joback Method
cpg	382.12	J/molxK	666.85	Joback Method
cpg	395.53	J/molxK	704.56	Joback Method
cpg	408.03	J/molxK	742.26	Joback Method

dvisc	0.0018157	Paxs	289.42	Joback Method
dvisc	0.0012161	Paxs	327.19	Joback Method
dvisc	0.0008849	Paxs	364.96	Joback Method
dvisc	0.0006835	Paxs	402.73	Joback Method
dvisc	0.0005518	Paxs	440.49	Joback Method
dvisc	0.0004608	Paxs	478.26	Joback Method
dvisc	0.0003951	Paxs	516.03	Joback Method

Sources

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=R256685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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