

1,3,4-trimethyl-isochroman, 1e',3e, 4a'

Inchi:	InChI=1S/C12H16O/c1-8-9(2)13-10(3)12-7-5-4-6-11(8)12/h4-10H,1-3H3/t8-,9-,10+/m1/s-
InchiKey:	VGXUJWDOBIUFTF-BBBLIVSA-N
Formula:	C12H16O
SMILES:	CC1OC(C)C(C)c2ccccc21
Mol. weight [g/mol]:	176.25

Physical Properties

Property code	Value	Unit	Source
gf	100.05	kJ/mol	Joback Method
hf	-171.99	kJ/mol	Joback Method
hfus	26.64	kJ/mol	Joback Method
hvap	49.22	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.270		Crippen Method
mcvol	151.190	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1288.00		NIST Webbook
rinpol	1288.00		NIST Webbook
ripol	1705.30		NIST Webbook
tb	534.24	K	Joback Method
tc	756.37	K	Joback Method
tf	296.45	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.44	J/molxK	534.24	Joback Method
cpg	385.17	J/molxK	571.26	Joback Method
cpg	402.78	J/molxK	608.28	Joback Method
cpg	419.31	J/molxK	645.31	Joback Method
cpg	434.81	J/molxK	682.33	Joback Method
cpg	449.31	J/molxK	719.35	Joback Method
cpg	462.86	J/molxK	756.37	Joback Method

dvisc	0.0015056	Paxs	296.45	Joback Method
dvisc	0.0010730	Paxs	336.08	Joback Method
dvisc	0.0008213	Paxs	375.71	Joback Method
dvisc	0.0006616	Paxs	415.35	Joback Method
dvisc	0.0005534	Paxs	454.98	Joback Method
dvisc	0.0004763	Paxs	494.61	Joback Method
dvisc	0.0004192	Paxs	534.24	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=R256665&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
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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