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

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+/m0/s
InchiKey: VGXUJWDOBIUFTF-IVZWLZJFSA-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	1301.40		NIST Webbook
rinpol	1301.40		NIST Webbook
ripol	1746.70		NIST Webbook
ripol	1746.70		NIST Webbook
tb	534.24	K	Joback Method
tc	756.37	K	Joback Method
tf	296.45	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	462.86	J/mol×K	756.37	Joback Method
dvisc	0.0004192	Pa×s	534.24	Joback Method
dvisc	0.0004763	Pa×s	494.61	Joback Method
dvisc	0.0005534	Pa×s	454.98	Joback Method
dvisc	0.0006616	Pa×s	415.35	Joback Method
dvisc	0.0008213	Pa×s	375.71	Joback Method
dvisc	0.0010730	Pa×s	336.08	Joback Method
dvisc	0.0015056	Pa×s	296.45	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=R256650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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