3,4-dimethyl-isochroman, 3e, 4a

Inchi: InChI=1S/C11H14O/c1-8-9(2)12-7-10-5-3-4-6-11(8)10/h3-6,8-9H,7H2,1-2H3/t8-,9-/m1/s1
InchiKey: FPFYZFBSRBZAHR-RKDXNWHRSA-N
Formula: C11H14O
SMILES: CC1OCc2ccccc2C1C
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	1274.00		NIST Webbook
ripol	1756.10		NIST Webbook
tb	516.03	K	Joback Method
tc	742.26	K	Joback Method
tf	289.42	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.39	J/mol×K	516.03	Joback Method
cpg	335.94	J/mol×K	553.74	Joback Method
cpg	352.37	J/mol×K	591.44	Joback Method
cpg	367.75	J/mol×K	629.15	Joback Method
cpg	382.12	J/mol×K	666.85	Joback Method
cpg	395.53	J/mol×K	704.56	Joback Method
cpg	408.03	J/mol×K	742.26	Joback Method
dvisc	0.0018157	Pa×s	289.42	Joback Method

dvisc	0.0012161	Pa×s	327.19	Joback Method
dvisc	0.0008849	Pa×s	364.96	Joback Method
dvisc	0.0006835	Pa×s	402.73	Joback Method
dvisc	0.0005518	Pa×s	440.49	Joback Method
dvisc	0.0004608	Pa×s	478.26	Joback Method
dvisc	0.0003951	Pa×s	516.03	Joback Method

Sources

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=R256734&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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