2H-1-Benzopyran, 3,4-dihydro-2,2-dimethyl-

Other names: Chroman, 2,2-dimethyl-
2,2-Dimethylchroman
Inchi: InChI=1S/C11H14O/c1-11(2)8-7-9-5-3-4-6-10(9)12-11/h3-6H,7-8H2,1-2H3
InchiKey: MITIYLBEZOKYLX-UHFFFAOYSA-N
Formula: C11H14O
SMILES: CC1(C)CCc2ccccc2O1
Mol. weight [g/mol]: 162.23
CAS: 1198-96-5

Physical Properties

Property code	Value	Unit	Source
gf	101.56	kJ/mol	Joback Method
hf	-95.43	kJ/mol	Joback Method
hfus	15.61	kJ/mol	Joback Method
hvap	46.46	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.790		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	520.94	K	Joback Method
tc	757.18	K	Joback Method
tf	317.56	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.22	J/mol×K	520.94	Joback Method
cpg	334.13	J/mol×K	560.31	Joback Method
cpg	349.73	J/mol×K	599.69	Joback Method
cpg	364.17	J/mol×K	639.06	Joback Method
cpg	377.65	J/mol×K	678.44	Joback Method
cpg	390.33	J/mol×K	717.81	Joback Method
cpg	402.39	J/mol×K	757.18	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.70	K	1.50	NIST Webbook

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=C1198965&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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume