2H-1-Benzopyran, 2,2-dimethyl-

Other names: 2,2-Dimethylchromene
2,2-Dimethylbenzopyran
Inchi: InChI=1S/C11H12O/c1-11(2)8-7-9-5-3-4-6-10(9)12-11/h3-8H,1-2H3
InchiKey: SAXKWTPDZMBKSQ-UHFFFAOYSA-N
Formula: C11H12O
SMILES: CC1(C)C=Cc2ccccc2O1
Mol. weight [g/mol]: 160.21
CAS: 2513-25-9

Physical Properties

Property code	Value	Unit	Source
gf	131.52	kJ/mol	Joback Method
hf	-37.65	kJ/mol	Joback Method
hfus	16.84	kJ/mol	Joback Method
hvap	46.75	kJ/mol	Joback Method
ie	7.80 ± 0.10	eV	NIST Webbook
log10ws	-3.26		Crippen Method
logp	2.871		Crippen Method
mcvol	132.800	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
tb	520.10	K	Joback Method
tc	758.83	K	Joback Method
tf	318.32	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.53	J/mol×K	520.10	Joback Method
cpg	315.11	J/mol×K	559.89	Joback Method
cpg	329.40	J/mol×K	599.68	Joback Method
cpg	342.58	J/mol×K	639.46	Joback Method
cpg	354.84	J/mol×K	679.25	Joback Method
cpg	366.36	J/mol×K	719.04	Joback Method

cpg	377.32	J/mol×K	758.83	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.20	K	1.50	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2513259&Units=SI

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
ie: Ionization energy
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