trans-Chrysanthenol

Other names: trans-Chrysanthenyl alcohol
(E)-Chrysanthenole
Inchi: InChI=1S/C10H16O/c1-6-4-5-7-9(11)8(6)10(7,2)3/h4,7-9,11H,5H2,1-3H3
InchiKey: IRZWAJHUWGZMMT-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1=CCC2C(O)C1C2(C)C
Mol. weight [g/mol]: 152.23
CAS: 38043-83-3

Physical Properties

Property code	Value	Unit	Source
gf	5.32	kJ/mol	Joback Method
hf	-241.65	kJ/mol	Joback Method
hfus	16.59	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1121.40		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1121.40		NIST Webbook
tb	533.17	K	Joback Method
tc	729.30	K	Joback Method
tf	324.34	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.85	J/mol×K	533.17	Joback Method
cpg	351.53	J/mol×K	565.86	Joback Method
cpg	365.30	J/mol×K	598.55	Joback Method
cpg	378.26	J/mol×K	631.23	Joback Method
cpg	390.53	J/mol×K	663.92	Joback Method
cpg	402.21	J/mol×K	696.61	Joback Method
cpg	413.40	J/mol×K	729.30	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=C38043833&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume