

trans-Chrysanthenyl acetate

Other names:	(E)-Chrysanthenyl acetate trans -Crysanthenyl acetate
Inchi:	InChI=1S/C12H18O2/c1-7-5-6-9-11(14-8(2)13)10(7)12(9,3)4/h5,9-11H,6H2,1-4H3
InchiKey:	UASZOTVHPVEMQR-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CC(=O)OC1C2CC=C(C)C1C2(C)C
Mol. weight [g/mol]:	194.27
CAS:	54324-99-1

Physical Properties

Property code	Value	Unit	Source
gf	-74.94	kJ/mol	Joback Method
hf	-375.50	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Joback Method
hvap	50.64	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1228.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1235.00		NIST Webbook

rinpol	1235.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1235.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1534.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1538.00		NIST Webbook
tb	563.04	K	Joback Method
tc	773.40	K	Joback Method
tf	358.22	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.92	J/mol×K	563.04	Joback Method
cpg	437.32	J/mol×K	598.10	Joback Method
cpg	453.71	J/mol×K	633.16	Joback Method
cpg	469.20	J/mol×K	668.22	Joback Method
cpg	483.90	J/mol×K	703.28	Joback Method
cpg	497.94	J/mol×K	738.34	Joback Method
cpg	511.43	J/mol×K	773.40	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=C54324991&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
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

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