(+)-cis-rose oxide

Other names: 2H-Pyran, tetrahydro-4-methyl-2-(2-methyl-1-propenyl)-, (2R,4S)-rel-
cis-Rose oxide
Inchi: InChI=1S/C10H18O/c1-8(2)6-10-7-9(3)4-5-11-10/h6,9-10H,4-5,7H2,1-3H3
InchiKey: CZCBTSFUTPZVKJ-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC(C)=CC1CC(C)CCO1
Mol. weight [g/mol]: 154.25
CAS: 876-17-5

Physical Properties

Property code	Value	Unit	Source
gf	35.61	kJ/mol	Joback Method
hf	-240.32	kJ/mol	Joback Method
hfus	21.43	kJ/mol	Joback Method
hvap	42.52	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.768		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1111.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1109.00		NIST Webbook

rinpol	1107.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1102.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1128.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1102.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1121.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1098.00	NIST Webbook
ripol	1358.00	NIST Webbook
ripol	1337.00	NIST Webbook
ripol	1368.00	NIST Webbook
ripol	1331.00	NIST Webbook
ripol	1358.00	NIST Webbook
ripol	1337.00	NIST Webbook
ripol	1364.00	NIST Webbook
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ripol	1362.00	NIST Webbook
ripol	1358.00	NIST Webbook
ripol	1331.00	NIST Webbook
ripol	1348.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1369.00	NIST Webbook
ripol	1344.00	NIST Webbook
ripol	1349.00	NIST Webbook
ripol	1354.00	NIST Webbook

ripol	1355.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1346.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1345.00		NIST Webbook
tb	474.07	K	Joback Method
tc	683.76	K	Joback Method
tf	213.13	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.04	J/mol×K	474.07	Joback Method
cpg	337.36	J/mol×K	509.02	Joback Method
cpg	355.66	J/mol×K	543.97	Joback Method
cpg	372.96	J/mol×K	578.92	Joback Method
cpg	389.30	J/mol×K	613.87	Joback Method
cpg	404.72	J/mol×K	648.81	Joback Method
cpg	419.25	J/mol×K	683.76	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C876175&Units=SI
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

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