trans-Rose oxide

Other names:	(E)-Rose oxide
	Rose oxide, II
	(t)-Rose oxide
	2H-Pyran, tetrahydro-4-methyl-2-(2-methyl-1-propenyl)-, (2R,4R)-rel-
	trans-Rose oxide
	Rose oxide trans
Inchi:	InChI=1S/C10H18O/c1-8(2)6-10-7-9(3)4-5-11-10/h6,9-10H,4-5,7H2,1-3H3/t9-,10+/m0/s1
InchiKey:	CZCBTSFUTPZVKJ-VHSXEESVSA-N
Formula:	C10H18O
SMILES:	CC(C)=CC1CC(C)CCO1
Mol. weight [g/mol]:	154.25
CAS:	876-18-6

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	1107.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1116.00		NIST Webbook

rinpol	1115.00	NIST Webbook
rinpol	1128.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1127.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1127.00	NIST Webbook
rinpol	1079.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1130.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1116.00	NIST Webbook
ripol	1417.00	NIST Webbook
ripol	1383.00	NIST Webbook
ripol	1365.00	NIST Webbook
ripol	1386.00	NIST Webbook
ripol	1358.00	NIST Webbook
ripol	1341.00	NIST Webbook
ripol	1362.00	NIST Webbook
ripol	1341.00	NIST Webbook
ripol	1350.00	NIST Webbook
ripol	1341.00	NIST Webbook
ripol	1370.00	NIST Webbook
ripol	1367.00	NIST Webbook
ripol	1355.00	NIST Webbook
ripol	1371.00	NIST Webbook
ripol	1367.00	NIST Webbook
ripol	1341.00	NIST Webbook
ripol	1366.00	NIST Webbook
ripol	1370.00	NIST Webbook
ripol	1379.00	NIST Webbook
ripol	1341.00	NIST Webbook
ripol	1383.00	NIST Webbook

ripol	1365.00		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

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=C5258117&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume