2H-Pyran, tetrahydro-4-methyl-2-(2-methyl-1-propenyl)-

Other names: Rose oxide
2H-Pyran, tetrahydro-4-methyl-2-(2-methylpropenyl)-
Rosoxide
Rose oxide L
Pyran, tetrahydro-2-(2-methyl-1-propenyl)-4-methyl-
Pyran, 2-(2-methyl-1-propenyl)-4-methyltetrahydro-
4-Methyl-2-(2-methyl-1-propenyl)tetrahydro-2H-pyran
Rosenoxide
Tetrahydro-4-methyl-2-[2-methyl-1-propenyl]-2H-pyran
2H-Pyran, tetrahydro-4-methyl-2-(2-methyl-1-propen-1-yl)-
Pyran, tetrahydro-4-methyl-2-(2-methylpropenyl)-
Rose oxide , I
tetrahydro-4-methyl-2-(2-methylprop-1-enyl)pyran

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-/m1/s1

InchiKey: CZCBTSFUTPZVKJ-NXEZZACHSA-N

Formula: C10H18O

SMILES: CC(C)=CC1CC(C)CCO1

Mol. weight [g/mol]: 154.25

CAS: 16409-43-1

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	1108.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1100.00		NIST Webbook

rinpol	1115.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1112.70		NIST Webbook
rinpol	1112.70		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1112.30		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1350.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16409431&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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