

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-
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:	<chem>CC(C)=CC1CC(C)CCO1</chem>
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	1115.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1079.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1341.00		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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.04	J/molxK	474.07	Joback Method
cpg	337.36	J/molxK	509.02	Joback Method
cpg	355.66	J/molxK	543.97	Joback Method
cpg	372.96	J/molxK	578.92	Joback Method
cpg	389.30	J/molxK	613.87	Joback Method
cpg	404.72	J/molxK	648.81	Joback Method
cpg	419.25	J/molxK	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=C876186&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
ripol:	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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