

Retinal, 9-cis-

Other names:	Isoretinene a 9-cis-Retinal 9-cis-Retinaldehyde 9-cis-Vitamin A Aldehyde 9-cis-3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraenal
Inchi:	InChI=1S/C20H28O/c1-16(8-6-9-17(2)13-15-21)11-12-19-18(3)10-7-14-20(19,4)5/h6,8-9
InchiKey:	NCYCYZXNIZJOKI-MKOSUFFBSA-N
Formula:	C20H28O
SMILES:	<chem>CC(C=CC=C(C)C=CC1=C(C)CCCC1(C)C)=CC=O</chem>
Mol. weight [g/mol]:	284.44
CAS:	514-85-2

Physical Properties

Property code	Value	Unit	Source
gf	351.44	kJ/mol	Joback Method
hf	11.99	kJ/mol	Joback Method
hfus	34.01	kJ/mol	Joback Method
hvap	67.72	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.717		Crippen Method
mcvol	261.870	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	2198.00		NIST Webbook
rinpol	2198.00		NIST Webbook
rinpol	2198.00		NIST Webbook
tb	750.97	K	Joback Method
tc	972.13	K	Joback Method
tf	366.00	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.66	J/molxK	750.97	Joback Method

cpg	767.45	J/mol×K	787.83	Joback Method
cpg	786.54	J/mol×K	824.69	Joback Method
cpg	805.14	J/mol×K	861.55	Joback Method
cpg	823.44	J/mol×K	898.41	Joback Method
cpg	841.67	J/mol×K	935.27	Joback Method
cpg	860.01	J/mol×K	972.13	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=C514852&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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