

Rhodopin

Other names:	«psi», «psi»-Carotene, 1,2-dihydro-1-hydroxy-Lycopene, 1,2-dihydro-1-hydroxy-Lycopene, 1,2-dihydro-1-hydroxy-, all-trans-Rhodopin, all-trans-
Inchi:	InChI=1S/C40H58O/c1-33(2)19-13-22-36(5)25-16-28-37(6)26-14-23-34(3)20-11-12-21-3
InchiKey:	CNYVJTJLUKKCGM-RGGGOQHISA-N
Formula:	C40H58O
SMILES:	<chem>CC(C)=CCCC(C)=CC=CC(C)=CC=CC(C)=CC=CC=C(C)C=CC=C(C)C=CC=C(C)CCCC</chem>
Mol. weight [g/mol]:	554.89
CAS:	105-92-0

Physical Properties

Property code	Value	Unit	Source
gf	1054.73	kJ/mol	Joback Method
hf	308.20	kJ/mol	Joback Method
hfus	89.28	kJ/mol	Joback Method
hvap	120.07	kJ/mol	Joback Method
log10ws	-14.19		Crippen Method
logp	12.133		Crippen Method
mcvol	528.730	ml/mol	McGowan Method
pc	543.86	kPa	Joback Method
rinpol	4025.00		NIST Webbook
tb	1252.63	K	Joback Method
tc	1568.57	K	Joback Method
tf	445.12	K	Joback Method
vc	2.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1963.74	J/molxK	1252.63	Joback Method
cpg	2021.82	J/molxK	1305.29	Joback Method
cpg	2085.66	J/molxK	1357.94	Joback Method
cpg	2156.27	J/molxK	1410.60	Joback Method

cpg	2234.62	J/mol×K	1463.26	Joback Method
cpg	2321.71	J/mol×K	1515.91	Joback Method
cpg	2418.52	J/mol×K	1568.57	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=C105920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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