Oxirane, 2,2-dimethyl-3-(3,7,12,16,20-pentamethyl-3,7,11,15-(all-E)-

Other names: 2,2-Dimethyl-3-((3E,7E,11E,15E)-3,7,12,16,20-pentamethylhenicosa-3,7,11,15,19-pentae
Inchi: InChI=1S/C30H50O/c1-24(2)14-11-17-27(5)20-12-18-25(3)15-9-10-16-26(4)19-13-21-28
InchiKey: QYIMSPSDBYKPPY-BANQPHDMSA-N
Formula: C30H50O
SMILES: CC(C)=CCCC(C)=CCCC(C)=CCCC=C(C)CCC=C(C)CCC1OC1(C)C
Mol. weight [g/mol]: 426.72
CAS: 7200-26-2

Physical Properties

Property code	Value	Unit	Source
gf	521.50	kJ/mol	Joback Method
hf	-189.68	kJ/mol	Joback Method
hfus	68.80	kJ/mol	Joback Method
hvap	85.53	kJ/mol	Joback Method
log10ws	-10.85		Crippen Method
logp	9.816		Crippen Method
mcvol	407.070	ml/mol	McGowan Method
pc	738.42	kPa	Joback Method
rinpol	2963.40		NIST Webbook
rinpol	2963.40		NIST Webbook
tb	935.26	K	Joback Method
tc	1146.41	K	Joback Method
tf	396.83	K	Joback Method
vc	1.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1375.92	J/mol×K	935.26	Joback Method
cpg	1403.12	J/mol×K	970.45	Joback Method
cpg	1430.44	J/mol×K	1005.64	Joback Method
cpg	1458.14	J/mol×K	1040.84	Joback Method
cpg	1486.46	J/mol×K	1076.03	Joback Method
cpg	1515.65	J/mol×K	1111.22	Joback Method

cpg	1545.96	J/mol×K	1146.41	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=C7200262&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume