

Retinoic acid, methyl ester

Other names:	Retinoic acid, methyl ester, all-trans- All-trans-Vitamin A acid methyl ester Methyl retinoate Ro 4-3781 Vitamin A acid methyl ester
Inchi:	InChI=1S/C21H30O2/c1-16(9-7-10-17(2)15-20(22)23-6)12-13-19-18(3)11-8-14-21(19,4)5
InchiKey:	SREQLAJQLXPNMC-DXYSAURFSA-N
Formula:	C21H30O2
SMILES:	COC(=O)C=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]:	314.46
CAS:	339-16-2

Physical Properties

Property code	Value	Unit	Source
gf	225.46	kJ/mol	Joback Method
hf	-167.87	kJ/mol	Joback Method
hfus	37.10	kJ/mol	Joback Method
hvap	72.38	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.691		Crippen Method
mcvol	281.830	ml/mol	McGowan Method
pc	1357.63	kPa	Joback Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
tb	801.48	K	Joback Method
tc	1021.53	K	Joback Method
tf	407.43	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.85	J/mol×K	801.48	Joback Method

cpg	857.14	J/mol×K	838.16	Joback Method
cpg	876.86	J/mol×K	874.83	Joback Method
cpg	896.19	J/mol×K	911.51	Joback Method
cpg	915.34	J/mol×K	948.18	Joback Method
cpg	934.47	J/mol×K	984.86	Joback Method
cpg	953.78	J/mol×K	1021.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C339162&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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