Squalene

Other names: (2E,6E,10E,14E,18E,22E)-2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaen
(6E,10E,14E,18E)-2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene
(All-E)-2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene
(E,E,E,E)-Squalene
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (2E,6E,10E,14E,18E)-
2,6,10,14,18,22-tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-
2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-Tetracosahexaene
2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene-, (all trans)-
2,6,10,15,19,23-Hexamethyltetracosa-2,6,10,14,18,22-hexaene
2,6,10,15,19,23-Hexamethyltetracosa-2,6,10,14,18,22-hexaene, (all E)-
2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene (all E)
Nikko Squalane EX
Spinacen
Spinacene
Squalen
Super Squalene
Supraene
all-trans-Squalene
trans-Spinacene
trans-Squalene

Inchi: InChI=1S/C30H50/c1-25(2)15-11-19-29(7)23-13-21-27(5)17-9-10-18-28(6)22-14-24-30(8

InchiKey: YYGNTYWPHWGJRM-AAJYLUCBSA-N

Formula: C30H50

SMILES: CC(C)=CCCC(C)=CCCC(C)=CCCC=C(C)CCC=C(C)CCC=C(C)C

Mol. weight [g/mol]: 410.72

CAS: 111-02-4

Physical Properties

Property code	Value	Unit	Source
gf	631.74	kJ/mol	Joback Method
hf	-17.95	kJ/mol	Joback Method
hfus	66.81	kJ/mol	Joback Method
hvap	82.60	kJ/mol	Joback Method
log10ws	-11.50		Crippen Method
logp	10.605		Crippen Method
mcvol	407.760	ml/mol	McGowan Method
pc	708.84	kPa	Joback Method

rinpol	2832.00		NIST Webbook
rinpol	2847.10		NIST Webbook
rinpol	2847.10		NIST Webbook
rinpol	2833.00		NIST Webbook
rinpol	2814.00		NIST Webbook
rinpol	2819.00		NIST Webbook
rinpol	2835.80		NIST Webbook
ripol	2865.00		NIST Webbook
tb	910.04	K	Joback Method
tc	1115.64	K	Joback Method
tf	313.62	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1321.66	J/mol×K	910.04	Joback Method
cpg	1345.18	J/mol×K	944.31	Joback Method
cpg	1367.98	J/mol×K	978.57	Joback Method
cpg	1390.21	J/mol×K	1012.84	Joback Method
cpg	1412.03	J/mol×K	1047.11	Joback Method
cpg	1433.58	J/mol×K	1081.37	Joback Method
cpg	1455.02	J/mol×K	1115.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	558.20	K	3.30	NIST Webbook

Sources

High-Pressure Phase Equilibria of Squalene + Carbon Dioxide: New Data and Thermodynamic Modeling:	https://www.doi.org/10.1021/je1001939
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Corosolic Acid in Supercritical Carbon Dioxide and Its Representation Using Density-Based Correlations:	https://www.doi.org/10.1021/je101228k
High-Pressure Phase Equilibria of the Ternary System Oleic Acid + Squalene + Carbon Dioxide:	https://www.doi.org/10.1021/je060459u

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111024&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Phase Equilibrium of Hydrogen, Carbon Dioxide, Squalene, and Squalane:	https://www.doi.org/10.1021/je800926z
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of Squalene and Fatty Acids in Carbon Dioxide at Supercritical Conditions: Binary and Ternary Systems:	https://www.doi.org/10.1021/acs.jced.7b00620

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume