Supraene

Other names:	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl- Spinacene 2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene 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-UHFFFAOYSA-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:	7683-64-9

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	2838.00		NIST Webbook
rinpol	2834.00		NIST Webbook
rinpol	2838.00		NIST Webbook
rinpol	2817.00		NIST Webbook
rinpol	2831.10		NIST Webbook
rinpol	2815.40		NIST Webbook
rinpol	2822.00		NIST Webbook
rinpol	2818.00		NIST Webbook
rinpol	2797.00		NIST Webbook
rinpol	2803.00		NIST Webbook
rinpol	2805.00		NIST Webbook
rinpol	2828.00		NIST Webbook
rinpol	2834.00		NIST Webbook
rinpol	2812.00		NIST Webbook
rinpol	2829.00		NIST Webbook
rinpol	2795.30		NIST Webbook

rinpol	2823.00		NIST Webbook
rinpol	2828.00		NIST Webbook
rinpol	2790.00		NIST Webbook
rinpol	2808.00		NIST Webbook
rinpol	2839.00		NIST Webbook
rinpol	2835.00		NIST Webbook
rinpol	2829.00		NIST Webbook
rinpol	2828.00		NIST Webbook
rinpol	2817.00		NIST Webbook
rinpol	2835.00		NIST Webbook
rinpol	462.10		NIST Webbook
rinpol	463.00		NIST Webbook
rinpol	463.10		NIST Webbook
rinpol	454.30		NIST Webbook
rinpol	2803.00		NIST Webbook
rinpol	454.90		NIST Webbook
rinpol	462.40		NIST Webbook
rinpol	446.90		NIST Webbook
rinpol	2831.10		NIST Webbook
rinpol	459.40		NIST Webbook
ripol	3058.00		NIST Webbook
ripol	3062.00		NIST Webbook
ripol	3058.00		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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7683649&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume