1-Phytene

Other names: phyt-1-ene
3,7,11,15-Tetramethyl-1-hexadecene (1-phytene)
Inchi: InChI=1S/C20H40/c1-7-18(4)12-9-14-20(6)16-10-15-19(5)13-8-11-17(2)3/h7,17-20H,1,8-
InchiKey: XQNRAQZFPXUCOT-UHFFFAOYSA-N
Formula: C20H40
SMILES: C=CC(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 280.53

Physical Properties

Property code	Value	Unit	Source
gf	195.60	kJ/mol	Joback Method
hf	-351.82	kJ/mol	Joback Method
hfus	32.18	kJ/mol	Joback Method
hvap	57.89	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	7.248		Crippen Method
mcvol	288.360	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1833.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1833.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1795.00		NIST Webbook
ripol	1850.00		NIST Webbook
tb	651.92	K	Joback Method
tc	821.40	K	Joback Method
tf	253.40	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.17	J/mol×K	651.92	Joback Method
cpg	839.77	J/mol×K	680.17	Joback Method
cpg	860.41	J/mol×K	708.41	Joback Method
cpg	880.11	J/mol×K	736.66	Joback Method
cpg	898.91	J/mol×K	764.90	Joback Method
cpg	916.84	J/mol×K	793.15	Joback Method
cpg	933.93	J/mol×K	821.40	Joback Method
dvisc	0.0185442	Pa×s	253.40	Joback Method
dvisc	0.0028626	Pa×s	319.82	Joback Method
dvisc	0.0008402	Pa×s	386.24	Joback Method
dvisc	0.0003534	Pa×s	452.66	Joback Method
dvisc	0.0001855	Pa×s	519.08	Joback Method
dvisc	0.0001127	Pa×s	585.50	Joback Method
dvisc	0.0000758	Pa×s	651.92	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R70567&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
dvisc: Dynamic viscosity
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