

phyta-trans-2,cis-4-diene

Inchi:	InChI=1S/C20H38/c1-7-18(4)12-9-14-20(6)16-10-15-19(5)13-8-11-17(2)3/h7,9,12,17,19-
InchiKey:	VQQYVFHLBANXKS-SESNXTKRSA-N
Formula:	C20H38
SMILES:	CC=C(C)C=CCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	278.52

Physical Properties

Property code	Value	Unit	Source
gf	262.09	kJ/mol	Joback Method
hf	-247.32	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	7.168		Crippen Method
mcvol	284.060	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
ripol	1945.00		NIST Webbook
tb	663.88	K	Joback Method
tc	841.15	K	Joback Method
tf	246.04	K	Joback Method
vc	1.099	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.86	J/mol×K	663.88	Joback Method
cpg	821.09	J/mol×K	693.43	Joback Method
cpg	841.31	J/mol×K	722.97	Joback Method
cpg	860.57	J/mol×K	752.52	Joback Method
cpg	878.94	J/mol×K	782.06	Joback Method
cpg	896.45	J/mol×K	811.61	Joback Method
cpg	913.16	J/mol×K	841.15	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=R330986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/72-679-9/phyta-trans-2-cis-4-diene.pdf>

Generated by Cheméo on 2024-04-26 08:06:29.030738434 +0000 UTC m=+16408037.951315746.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.