

phyta-trans-3,trans-5-diene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H38/c1-7-18(4)12-9-14-20(6)16-10-15-19(5)13-8-11-17(2)3/h9,12,14,17,19

RVPWORJGDCKSNT-CEIOHHNKSA-N

C20H38

CCC(C)=CC=CC(C)CCCC(C)CCCC(C)C

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	1880.00		NIST Webbook
ripol	1880.00		NIST Webbook
tb	663.88	K	Joback Method
tc	841.15	K	Joback Method
tf	246.04	K	Joback Method
vc	1.099	m3/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=R330991&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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