

Guaia-3,7-diene

Inchi:	InChI=1S/C16H26/c1-11-6-8-13(16(3,4)5)10-15-12(2)7-9-14(11)15/h7-8,11,14-15H,6,9-1
InchiKey:	QAUZVGPDSDIYTH-UHFFFAOYSA-N
Formula:	C16H26
SMILES:	CC1=CCC2C(C)CC=C(C(C)(C)C)CC12
Mol. weight [g/mol]:	218.38

Physical Properties

Property code	Value	Unit	Source
gf	192.73	kJ/mol	Joback Method
hf	-189.08	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	52.03	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.971		Crippen Method
mcvol	205.980	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	1474.00		NIST Webbook
ripol	1811.00		NIST Webbook
tb	596.42	K	Joback Method
tc	816.40	K	Joback Method
tf	316.62	K	Joback Method
vc	0.773	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.25	J/mol×K	596.42	Joback Method
cpg	583.08	J/mol×K	633.08	Joback Method
cpg	605.39	J/mol×K	669.75	Joback Method
cpg	626.26	J/mol×K	706.41	Joback Method
cpg	645.78	J/mol×K	743.07	Joback Method
cpg	664.01	J/mol×K	779.74	Joback Method
cpg	681.03	J/mol×K	816.40	Joback Method
dvisc	0.0022427	Paxs	316.62	Joback Method

dvisc	0.0013038	Paxs	363.25	Joback Method
dvisc	0.0008576	Paxs	409.89	Joback Method
dvisc	0.0006145	Paxs	456.52	Joback Method
dvisc	0.0004684	Paxs	503.15	Joback Method
dvisc	0.0003738	Paxs	549.79	Joback Method
dvisc	0.0003090	Paxs	596.42	Joback Method

Sources

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=R327009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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

Latest version available from:

<https://www.chemeo.com/cid/74-098-2/Guaia-3-7-diene.pdf>

Generated by Cheméo on 2024-04-27 10:54:50.225399012 +0000 UTC m=+16504539.145976334.

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