Phenanthrene, 1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-7-(1-methylethyl)-, (4aS-trans)-

Other names: Podocarpa-8,11,13-triene, 13-isopropyl-
ar-Abietatriene
Abieta-8,11,13-triene
Abietane, dehydro-
Dehydroabietan
Dehydroabietane
Abietatriene
8,11,13-Abietatriene
Abitatriene

Inchi: InChI=1S/C20H30/c1-14(2)15-7-9-17-16(13-15)8-10-18-19(3,4)11-6-12-20(17,18)5/h7,9,

InchiKey: QUUCYKKMFLJLFS-QUCCMNQESA-N

Formula: C20H30

SMILES: CC(C)c1ccc2c(c1)CCC1C(C)(C)CCCC21C

Mol. weight [g/mol]: 270.45

CAS: 19407-28-4

Physical Properties

Property code	Value	Unit	Source
gf	286.84	kJ/mol	Joback Method
hf	-104.40	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	60.89	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.840		Crippen Method
mcvol	247.180	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2018.00		NIST Webbook
rinpol	2041.00		NIST Webbook
rinpol	2052.00		NIST Webbook
rinpol	2068.70		NIST Webbook
rinpol	2049.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	2027.00		NIST Webbook
rinpol	2027.00		NIST Webbook

rinpol	2057.00	NIST Webbook
rinpol	2078.00	NIST Webbook
rinpol	2057.00	NIST Webbook
rinpol	2057.00	NIST Webbook
rinpol	2054.00	NIST Webbook
rinpol	2073.00	NIST Webbook
rinpol	2055.00	NIST Webbook
rinpol	2054.00	NIST Webbook
rinpol	2078.00	NIST Webbook
rinpol	2027.00	NIST Webbook
rinpol	2072.00	NIST Webbook
rinpol	2075.00	NIST Webbook
rinpol	2051.00	NIST Webbook
rinpol	2019.00	NIST Webbook
rinpol	2019.00	NIST Webbook
rinpol	2013.00	NIST Webbook
rinpol	2034.00	NIST Webbook
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rinpol	2050.00	NIST Webbook
rinpol	2040.00	NIST Webbook
rinpol	2018.00	NIST Webbook
rinpol	2018.00	NIST Webbook
rinpol	2055.00	NIST Webbook
rinpol	2058.00	NIST Webbook
rinpol	2017.00	NIST Webbook
rinpol	2054.00	NIST Webbook
rinpol	2054.00	NIST Webbook
rinpol	2058.00	NIST Webbook
rinpol	2056.00	NIST Webbook

rinpol	2054.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2049.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2068.70		NIST Webbook
rinpol	2004.00		NIST Webbook
rinpol	2094.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	2039.00		NIST Webbook
rinpol	2021.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2049.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2044.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2030.00		NIST Webbook
ripol	2498.00		NIST Webbook
ripol	2482.00		NIST Webbook
ripol	2512.00		NIST Webbook
ripol	2476.00		NIST Webbook
ripol	2482.00		NIST Webbook
ripol	2488.00		NIST Webbook
ripol	2524.00		NIST Webbook
ripol	2530.00		NIST Webbook
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ripol	2498.00		NIST Webbook
ripol	2493.00		NIST Webbook
ripol	2530.00		NIST Webbook
ripol	2530.00		NIST Webbook
ripol	2489.00		NIST Webbook
ripol	2488.00		NIST Webbook
tb	711.03	K	Joback Method
tc	947.41	K	Joback Method

tf	424.02	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.09	J/mol×K	711.03	Joback Method
cpg	764.29	J/mol×K	750.43	Joback Method
cpg	787.63	J/mol×K	789.82	Joback Method
cpg	810.45	J/mol×K	829.22	Joback Method
cpg	833.07	J/mol×K	868.62	Joback Method
cpg	855.84	J/mol×K	908.01	Joback Method
cpg	879.08	J/mol×K	947.41	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19407284&Units=SI

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