Abietadiene

Other names: Abieta-7,13-diene
Abitadiene
7,13-abietadiene
Inchi: InChI=1S/C20H32/c1-14(2)15-7-9-17-16(13-15)8-10-18-19(3,4)11-6-12-20(17,18)5/h8,13
InchiKey: BBPXZLJCPUPNGH-UHFFFAOYSA-N
Formula: C20H32
SMILES: CC(C)C1=CC2=CCC3C(C)(C)CCCC3(C)C2CC1
Mol. weight [g/mol]: 272.47
CAS: 35241-40-8

Physical Properties

Property code	Value	Unit	Source
gf	258.80	kJ/mol	Joback Method
hf	-171.05	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hvap	59.62	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	6.142		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2064.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2107.20		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2080.00		NIST Webbook

rinpol	2073.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2061.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2044.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
ripol	2449.00		NIST Webbook
ripol	2449.00		NIST Webbook
ripol	2410.00		NIST Webbook
ripol	2447.00		NIST Webbook
ripol	2410.00		NIST Webbook
ripol	2450.00		NIST Webbook
tb	702.22	K	Joback Method
tc	935.86	K	Joback Method
tf	406.50	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.28	J/mol×K	702.22	Joback Method
cpg	792.08	J/mol×K	741.16	Joback Method
cpg	816.84	J/mol×K	780.10	Joback Method
cpg	840.88	J/mol×K	819.04	Joback Method
cpg	864.52	J/mol×K	857.98	Joback Method
cpg	888.08	J/mol×K	896.92	Joback Method
cpg	911.87	J/mol×K	935.86	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=C35241408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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