Abieta-7,13-dien-3-one

Other names: Abieta-7,13-diene-3-one
(4aR,4bR,10aR)-7-Isopropyl-1,1,4a-trimethyl-3,4,4a,4b,5,6,10,10a-octahydrophenanthren
Inchi: InChI=1S/C20H30O/c1-13(2)14-6-8-16-15(12-14)7-9-17-19(3,4)18(21)10-11-20(16,17)5/
InchiKey: BOPYLVIBVAFZAH-HLIPFELVSA-N
Formula: C20H30O
SMILES: CC(C)C1=CC2=CCC3C(C)(C)C(=O)CCC3(C)C2CC1
Mol. weight [g/mol]: 286.45
CAS: 29461-25-4

Physical Properties

Property code	Value	Unit	Source
gf	136.21	kJ/mol	Joback Method
hf	-308.75	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	63.87	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.321		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2313.00		NIST Webbook
rinpol	2302.00		NIST Webbook
rinpol	2313.00		NIST Webbook
rinpol	2297.00		NIST Webbook
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook
rinpol	2297.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2335.50		NIST Webbook
tb	770.04	K	Joback Method
tc	1013.89	K	Joback Method
tf	474.72	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.44	J/mol×K	770.04	Joback Method
cpg	835.91	J/mol×K	810.68	Joback Method
cpg	860.76	J/mol×K	851.32	Joback Method
cpg	885.32	J/mol×K	891.96	Joback Method
cpg	909.90	J/mol×K	932.60	Joback Method
cpg	934.82	J/mol×K	973.24	Joback Method
cpg	960.39	J/mol×K	1013.89	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=C29461254&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume