Abieta-8,11,13-trien-7-one

Inchi: InChI=1S/C20H28O/c1-13(2)14-7-8-16-15(11-14)17(21)12-18-19(3,4)9-6-10-20(16,18)5/
InchiKey: ISHVJVXYPLFKAL-UHFFFAOYSA-N
Formula: C20H28O
SMILES: CC(C)c1ccc2c(c1)C(=O)CC1C(C)(C)CCCC21C
Mol. weight [g/mol]: 284.44

Physical Properties

Property code	Value	Unit	Source
gf	164.25	kJ/mol	Joback Method
hf	-242.10	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	65.13	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.480		Crippen Method
mcvol	248.750	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2284.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2293.00		NIST Webbook
rinpol	2312.00		NIST Webbook
rinpol	2312.00		NIST Webbook
tb	778.85	K	Joback Method
tc	1025.29	K	Joback Method
tf	492.24	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.17	J/mol×K	778.85	Joback Method
cpg	805.28	J/mol×K	819.92	Joback Method
cpg	828.98	J/mol×K	861.00	Joback Method
cpg	852.60	J/mol×K	902.07	Joback Method
cpg	876.48	J/mol×K	943.14	Joback Method

cpg	900.94	J/mol×K	984.22	Joback Method
cpg	926.31	J/mol×K	1025.29	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=R290452&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume