Dehydroabietol benzoate

Inchi: InChI=1S/C27H34O2/c1-19(2)21-11-13-23-22(17-21)12-14-24-26(3,15-8-16-27(23,24)4)
InchiKey: XIPLYJCTZZOWRG-UHFFFAOYSA-N
Formula: C27H34O2
SMILES: CC(C)c1ccc2c(c1)CCC1C(C)(COC(=O)c3ccccc3)CCCC21C
Mol. weight [g/mol]: 390.56
CAS: 121974-96-7

Physical Properties

Property code	Value	Unit	Source
gf	224.27	kJ/mol	Joback Method
hf	-257.15	kJ/mol	Joback Method
hfus	32.80	kJ/mol	Joback Method
hvap	87.90	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.677		Crippen Method
mcvol	329.490	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	3078.60		NIST Webbook
rinpol	3078.60		NIST Webbook
tb	974.16	K	Joback Method
tc	1223.09	K	Joback Method
tf	601.49	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.66	J/mol×K	974.16	Joback Method
cpg	1172.56	J/mol×K	1015.65	Joback Method
cpg	1202.51	J/mol×K	1057.14	Joback Method
cpg	1233.90	J/mol×K	1098.63	Joback Method
cpg	1267.15	J/mol×K	1140.12	Joback Method
cpg	1302.66	J/mol×K	1181.61	Joback Method
cpg	1340.84	J/mol×K	1223.09	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=C121974967&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