Dehydroabietol cinnamate

Inchi: InChI=1S/C29H36O2/c1-21(2)23-12-14-25-24(19-23)13-15-26-28(3,17-8-18-29(25,26)4)2
InchiKey: RPKRJWSKXBIBJU-LFIBNONCSA-N
Formula: C29H36O2
SMILES: CC(C)c1ccc2c(c1)CCC1C(C)(COC(=O)C=Cc3ccccc3)CCCC21C
Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	321.33	kJ/mol	Joback Method
hf	-181.21	kJ/mol	Joback Method
hfus	38.18	kJ/mol	Joback Method
hvap	92.31	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	7.077		Crippen Method
mcvol	353.370	ml/mol	McGowan Method
pc	1191.52	kPa	Joback Method
rinpol	3391.50		NIST Webbook
rinpol	3391.50		NIST Webbook
tb	1024.08	K	Joback Method
tc	1275.06	K	Joback Method
tf	618.95	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.09	J/mol×K	1024.08	Joback Method
cpg	1284.26	J/mol×K	1065.91	Joback Method
cpg	1318.10	J/mol×K	1107.74	Joback Method
cpg	1354.08	J/mol×K	1149.57	Joback Method
cpg	1392.63	J/mol×K	1191.40	Joback Method
cpg	1434.22	J/mol×K	1233.23	Joback Method
cpg	1479.28	J/mol×K	1275.06	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=U414717&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