Hydroxy-copalic acid methyl ester

Inchi: InChI=1S/C21H34O3/c1-14(13-19(23)24-6)7-9-16-15(2)8-10-17-20(3,4)18(22)11-12-21(1
InchiKey: ZPIMNSSFJAWUGM-GRKUEHCHSA-N
Formula: C21H34O3
SMILES: C=C1CCC2C(C)(C)C(O)CCC2(C)C1CCC(C)=CC(=O)OC
Mol. weight [g/mol]: 334.49

Physical Properties

Property code	Value	Unit	Source
gf	-81.06	kJ/mol	Joback Method
hf	-591.71	kJ/mol	Joback Method
hfus	33.24	kJ/mol	Joback Method
hvap	85.66	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.656		Crippen Method
mcvol	289.740	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
tb	868.58	K	Joback Method
tc	1079.40	K	Joback Method
tf	510.93	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.14	J/mol×K	868.58	Joback Method
cpg	1004.81	J/mol×K	903.72	Joback Method
cpg	1027.45	J/mol×K	938.85	Joback Method
cpg	1050.27	J/mol×K	973.99	Joback Method
cpg	1073.47	J/mol×K	1009.13	Joback Method
cpg	1097.27	J/mol×K	1044.27	Joback Method
cpg	1121.87	J/mol×K	1079.40	Joback Method

Sources

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=R519401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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