trans-Verbenyl laureate

Inchi: InChI=1S/C22H38O2/c1-5-6-7-8-9-10-11-12-13-14-21(23)24-20-15-17(2)18-16-19(20)22
InchiKey: HALFTOAKQHSZDB-UHFFFAOYSA-N
Formula: C22H38O2
SMILES: CCCCCCCCCCCC(=O)OC1C=C(C)C2CC1C2(C)C
Mol. weight [g/mol]: 334.54

Physical Properties

Property code	Value	Unit	Source
gf	9.26	kJ/mol	Joback Method
hf	-581.90	kJ/mol	Joback Method
hfus	46.37	kJ/mol	Joback Method
hvap	72.91	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.441		Crippen Method
mcvol	302.260	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2276.60		NIST Webbook
rinpol	2276.60		NIST Webbook
tb	791.84	K	Joback Method
tc	983.74	K	Joback Method
tf	470.92	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.49	J/mol×K	791.84	Joback Method
cpg	1000.99	J/mol×K	823.82	Joback Method
cpg	1021.75	J/mol×K	855.81	Joback Method
cpg	1041.91	J/mol×K	887.79	Joback Method
cpg	1061.56	J/mol×K	919.78	Joback Method
cpg	1080.83	J/mol×K	951.76	Joback Method
cpg	1099.82	J/mol×K	983.74	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=U414148&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