

Myrtenyl laureate

Inchi:

InChI=1S/C22H38O2/c1-4-5-6-7-8-9-10-11-12-13-21(23)24-17-18-14-15-19-16-20(18)22

InchiKey:

QOZRLWRYYCENZEX-UHFFFAOYSA-N

Formula:

C22H38O2

SMILES:

CCCCCCCCCCCC(=O)OCC1=CCC2CC1C2(C)C

Mol. weight [g/mol]:

334.54

Physical Properties

Property code	Value	Unit	Source
gf	16.97	kJ/mol	Joback Method
hf	-561.56	kJ/mol	Joback Method
hfus	45.30	kJ/mol	Joback Method
hvap	73.21	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	6.443		Crippen Method
mcvol	302.260	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	2335.60		NIST Webbook
rinpol	2335.60		NIST Webbook
tb	796.51	K	Joback Method
tc	988.86	K	Joback Method
tf	475.16	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.94	J/mol×K	796.51	Joback Method
cpg	998.12	J/mol×K	828.57	Joback Method
cpg	1018.62	J/mol×K	860.63	Joback Method
cpg	1038.56	J/mol×K	892.68	Joback Method
cpg	1058.05	J/mol×K	924.74	Joback Method
cpg	1077.22	J/mol×K	956.80	Joback Method
cpg	1096.18	J/mol×K	988.86	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=U414142&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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