

trans-Pinocarvyl laureate

Inchi:	InChI=1S/C22H38O2/c1-5-6-7-8-9-10-11-12-13-14-21(23)24-20-16-18-15-19(17(20)2)22
InchiKey:	BQJZDGHPWPPVLY-UHFFFAOYSA-N
Formula:	C22H38O2
SMILES:	<chem>C=C1C(OC(=O)CCCCCCCCC)CC2CC1C2(C)C</chem>
Mol. weight [g/mol]:	334.54

Physical Properties

Property code	Value	Unit	Source
gf	42.01	kJ/mol	Joback Method
hf	-543.97	kJ/mol	Joback Method
hfus	44.38	kJ/mol	Joback Method
hvap	72.11	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.441		Crippen Method
mvol	302.260	ml/mol	McGowan Method
pc	1110.37	kPa	Joback Method
rinpol	2302.20		NIST Webbook
rinpol	2302.20		NIST Webbook
tb	786.86	K	Joback Method
tc	977.82	K	Joback Method
tf	471.32	K	Joback Method
vc	1.177	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.43	J/molxK	786.86	Joback Method
cpg	1000.01	J/molxK	818.69	Joback Method
cpg	1020.83	J/molxK	850.51	Joback Method
cpg	1041.01	J/molxK	882.34	Joback Method
cpg	1060.66	J/molxK	914.17	Joback Method
cpg	1079.88	J/molxK	946.00	Joback Method
cpg	1098.79	J/molxK	977.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U414144&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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