

Senkyunone

Inchi:	InChI=1S/C22H30O2/c1-16(2)8-6-9-17(3)10-7-11-18(4)12-13-20-15-21(23)14-19(5)22(20)
InchiKey:	WJKQTIOYPPFGQW-VZRGJMDUSA-N
Formula:	C22H30O2
SMILES:	<chem>CC(C)=CCCC(C)=CCCC(C)=CCC1=CC(=O)C=C(C)C1=O</chem>
Mol. weight [g/mol]:	326.47
CAS:	142182-61-4

Physical Properties

Property code	Value	Unit	Source
gf	177.01	kJ/mol	Joback Method
hf	-283.24	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	75.82	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.820		Crippen Method
mvol	291.620	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	2536.80		NIST Webbook
rinpol	2536.80		NIST Webbook
tb	883.02	K	Joback Method
tc	1108.39	K	Joback Method
tf	455.20	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.03	J/mol×K	883.02	Joback Method
cpg	935.30	J/mol×K	920.58	Joback Method
cpg	952.28	J/mol×K	958.14	Joback Method
cpg	968.04	J/mol×K	995.70	Joback Method
cpg	982.62	J/mol×K	1033.27	Joback Method
cpg	996.08	J/mol×K	1070.83	Joback Method
cpg	1008.47	J/mol×K	1108.39	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=C142182614&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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