

Selina-1,3,5(11)-trien-8-one

Inchi:	InChI=1S/C15H20O/c1-10(2)12-8-13-11(3)6-5-7-15(13,4)9-14(12)16/h5-8,10,12H,9H2,1-
InchiKey:	ZJWXBZANERDOCV-WFASDCNBSA-N
Formula:	C15H20O
SMILES:	CC1=CC=CC2(C)CC(=O)C(C(C)C)C=C12
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
gf	88.62	kJ/mol	Joback Method
hf	-209.31	kJ/mol	Joback Method
hfus	15.05	kJ/mol	Joback Method
hvap	54.41	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.680		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
tb	648.22	K	Joback Method
tc	887.17	K	Joback Method
tf	385.05	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.89	J/molxK	648.22	Joback Method
cpg	536.93	J/molxK	688.04	Joback Method
cpg	555.84	J/molxK	727.87	Joback Method
cpg	573.79	J/molxK	767.69	Joback Method
cpg	590.90	J/molxK	807.52	Joback Method
cpg	607.35	J/molxK	847.34	Joback Method
cpg	623.26	J/molxK	887.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R547936&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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