Oxidoselina-1,3,7(11)-trien-8-one

Inchi: InChI=1S/C15H20O2/c1-10-6-5-7-14(4)9-12(16)15(8-11(10)14)13(2,3)17-15/h5-7,11H,8-
InchiKey: LGXDZGLEPFLCIY-WPBUFGDCSA-N
Formula: C15H20O2
SMILES: CC1=CC=CC2(C)CC(=O)C3(CC12)OC3(C)C
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	38.77	kJ/mol	Joback Method
hf	-293.24	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	55.48	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.035		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1689.00		NIST Webbook
tb	669.75	K	Joback Method
tc	924.73	K	Joback Method
tf	478.36	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.27	J/mol×K	669.75	Joback Method
cpg	570.54	J/mol×K	712.25	Joback Method
cpg	590.28	J/mol×K	754.74	Joback Method
cpg	609.98	J/mol×K	797.24	Joback Method
cpg	630.17	J/mol×K	839.73	Joback Method
cpg	651.34	J/mol×K	882.23	Joback Method
cpg	674.01	J/mol×K	924.73	Joback Method

Sources

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=R430883&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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