Selina-4(15),7(11),8(9)-triene

Inchi: InChI=1S/C15H22/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h7,9,14H,3,5-6,8,10H2,1
InchiKey: KKLLWPPBHBDDQD-YSSOQSIOSA-N
Formula: C15H22
SMILES: C=C1CCCC2(C)C=CC(=C(C)C)CC12
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	262.98	kJ/mol	Joback Method
hf	-8.47	kJ/mol	Joback Method
hfus	15.25	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.645		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1433.00		NIST Webbook
ripol	1681.00		NIST Webbook
ripol	1681.00		NIST Webbook
tb	578.24	K	Joback Method
tc	806.39	K	Joback Method
tf	315.35	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.59	J/mol×K	578.24	Joback Method
cpg	501.10	J/mol×K	616.26	Joback Method
cpg	521.21	J/mol×K	654.29	Joback Method
cpg	540.12	J/mol×K	692.31	Joback Method
cpg	557.97	J/mol×K	730.34	Joback Method
cpg	574.96	J/mol×K	768.36	Joback Method
cpg	591.25	J/mol×K	806.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321021&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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