(-)-selina-4,11-diene

Inchi: InChI=1S/C16H28/c1-7-16(6)10-8-9-13(4)15(16)11-14(5)12(2)3/h14H,2,7-11H2,1,3-6H3
InchiKey: ZRINCZUYERVHLK-UHFFFAOYSA-N
Formula: C16H28
SMILES: C=C(C)C(C)CC1=C(C)CCCC1(C)CC
Mol. weight [g/mol]: 220.39

Physical Properties

Property code	Value	Unit	Source
gf	190.35	kJ/mol	Joback Method
hf	-158.81	kJ/mol	Joback Method
hfus	17.06	kJ/mol	Joback Method
hvap	51.13	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.505		Crippen Method
mcvol	216.840	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	1519.50		NIST Webbook
rinpol	1519.50		NIST Webbook
ripol	1702.00		NIST Webbook
tb	590.51	K	Joback Method
tc	794.95	K	Joback Method
tf	296.44	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.20	J/mol×K	590.51	Joback Method
cpg	585.59	J/mol×K	624.58	Joback Method
cpg	605.86	J/mol×K	658.66	Joback Method
cpg	625.13	J/mol×K	692.73	Joback Method
cpg	643.50	J/mol×K	726.81	Joback Method
cpg	661.08	J/mol×K	760.88	Joback Method
cpg	677.99	J/mol×K	794.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142066&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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