(-)-(4S,5R,7S)-7-epi-Eremophyla-1(10),8,11-triene

Inchi: InChI=1S/C15H22/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h7-9,12-13H,1,5-6,10H2,
InchiKey: DQPQHEZYSQLQOQ-UHFFFAOYSA-N
Formula: C15H22
SMILES: C=C(C)C1C=CC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]: 202.34
CAS: 190327-38-9

Physical Properties

Property code	Value	Unit	Source
gf	264.90	kJ/mol	Joback Method
hf	-17.34	kJ/mol	Joback Method
hfus	16.71	kJ/mol	Joback Method
hvap	48.69	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.501		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1507.70		NIST Webbook
rinpol	1507.00		NIST Webbook
tb	568.59	K	Joback Method
tc	795.68	K	Joback Method
tf	298.59	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.93	J/mol×K	568.59	Joback Method
cpg	502.32	J/mol×K	606.44	Joback Method
cpg	523.23	J/mol×K	644.29	Joback Method
cpg	542.85	J/mol×K	682.13	Joback Method
cpg	561.34	J/mol×K	719.98	Joback Method
cpg	578.86	J/mol×K	757.83	Joback Method
cpg	595.59	J/mol×K	795.68	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=C190327389&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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