Eudesma-2,4(15),11-triene

Inchi: InChI=1S/C15H22/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h5-6,13-14H,1,3,7-10H2
InchiKey: DDLAIUOYTHJYGD-NRXISQOPSA-N
Formula: C15H22
SMILES: C=C(C)C1CCC2(C)CC=CC(=C)C2C1
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	297.65	kJ/mol	Joback Method
hf	20.59	kJ/mol	Joback Method
hfus	14.72	kJ/mol	Joback Method
hvap	47.90	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.501		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
tb	563.61	K	Joback Method
tc	789.42	K	Joback Method
tf	298.99	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.45	J/mol×K	563.61	Joback Method
cpg	501.07	J/mol×K	601.24	Joback Method
cpg	522.22	J/mol×K	638.88	Joback Method
cpg	542.04	J/mol×K	676.51	Joback Method
cpg	560.71	J/mol×K	714.15	Joback Method
cpg	578.38	J/mol×K	751.78	Joback Method
cpg	595.23	J/mol×K	789.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R416718&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume