Eudesma-2,4,11-triene

Inchi:	InChI=1S/C15H22/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h5-6,13H,1,7-10H2,2-4H
InchiKey:	LGRISOGTKBAJPA-UHFFFAOYSA-N
Formula:	C15H22
SMILES:	C=C(C)C1CCC2(C)CC=CC(C)=C2C1
Mol. weight [g/mol]:	202.34
CAS:	82462-31-5

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	1478.60		NIST Webbook
rinpol	1478.60		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

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=C82462315&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

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