4(14),11-Eudesmadiene

Inchi: InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h13-14H,1,3,5-10H2,2,4
InchiKey: YOVSPTNQHMDJAG-YMAMQOFZSA-N
Formula: C15H24
SMILES: C=C(C)C1CCC2(C)CCCC(=C)C2C1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	267.69	kJ/mol	Joback Method
hf	-37.19	kJ/mol	Joback Method
hfus	13.50	kJ/mol	Joback Method
hvap	47.61	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1465.00		NIST Webbook
tb	564.45	K	Joback Method
tc	788.06	K	Joback Method
tf	298.23	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.99	J/mol×K	564.45	Joback Method
cpg	521.74	J/mol×K	601.72	Joback Method
cpg	543.99	J/mol×K	638.99	Joback Method
cpg	564.88	J/mol×K	676.25	Joback Method
cpg	584.58	J/mol×K	713.52	Joback Method
cpg	603.25	J/mol×K	750.79	Joback Method
cpg	621.03	J/mol×K	788.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R574304&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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