(-)-6,7-seco-Eudesm-7(11)-en-6-al

Inchi: InChI=1S/C15H26O/c1-12(2)7-5-9-15(4)10-6-8-13(3)14(15)11-16/h7,11,13-14H,5-6,8-10
InchiKey: VWOHYEGRTUNEJL-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC(C)=CCCC1(C)CCCC(C)C1C=O
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	51.11	kJ/mol	Joback Method
hf	-302.20	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.374		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
tb	605.75	K	Joback Method
tc	812.64	K	Joback Method
tf	304.57	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.18	J/mol×K	605.75	Joback Method
cpg	584.36	J/mol×K	640.23	Joback Method
cpg	604.41	J/mol×K	674.71	Joback Method
cpg	623.43	J/mol×K	709.19	Joback Method
cpg	641.53	J/mol×K	743.68	Joback Method
cpg	658.84	J/mol×K	778.16	Joback Method
cpg	675.47	J/mol×K	812.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R504395&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

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