«alpha»-11-Eudesmene

Inchi: InChI=1S/C15H26/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h12-14H,1,5-10H2,2-4H3
InchiKey: DJLBUNMUAZWONS-URGYJCLVSA-N
Formula: C15H26
SMILES: C=C(C)C1CCC2(C)CCCC(C)C2C1
Mol. weight [g/mol]: 206.37

Physical Properties

Property code	Value	Unit	Source
gf	206.90	kJ/mol	Joback Method
hf	-141.77	kJ/mol	Joback Method
hfus	15.73	kJ/mol	Joback Method
hvap	47.14	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.805		Crippen Method
mcvol	196.190	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook
tb	560.62	K	Joback Method
tc	782.23	K	Joback Method
tf	280.31	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.66	J/mol×K	560.62	Joback Method
cpg	544.19	J/mol×K	597.55	Joback Method
cpg	568.12	J/mol×K	634.49	Joback Method
cpg	590.60	J/mol×K	671.42	Joback Method
cpg	611.80	J/mol×K	708.36	Joback Method
cpg	631.86	J/mol×K	745.29	Joback Method
cpg	650.94	J/mol×K	782.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418165&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