Tricyclo[4.4.0.0(2,7)]dec-8-ene-3-methanol, «alpha»,«alpha»,6,8-tetramethyl-, stereoisomer

Other names: «alpha»-Copaen-11-ol
Tricyclo[4.4.0.0(2,7)]dec-8-ene-5-methanol, «alpha»,«alpha»,2,8-tetramethyl-, stereoisomer
«alpha»-Copaene-11-ol

Inchi: InChI=1S/C15H24O/c1-9-5-6-11-12-10(14(2,3)16)7-8-15(11,4)13(9)12/h5,10-13,16H,6-8

InchiKey: IKIHFZGZEWTHEQ-UHFFFAOYSA-N

Formula: C15H24O

SMILES: CC1=CCC2C3C(C(C)(C)O)CCC2(C)C13

Mol. weight [g/mol]: 220.35

CAS: 41370-56-3

Physical Properties

Property code	Value	Unit	Source
gf	111.01	kJ/mol	Joback Method
hf	-280.80	kJ/mol	Joback Method
hfus	20.26	kJ/mol	Joback Method
hvap	63.46	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1547.60		NIST Webbook
rinpol	1539.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2023.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2065.00		NIST Webbook
tb	651.08	K	Joback Method
tc	857.47	K	Joback Method
tf	401.05	K	Joback Method

vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.16	J/mol×K	651.08	Joback Method
cpg	596.62	J/mol×K	685.48	Joback Method
cpg	614.07	J/mol×K	719.88	Joback Method
cpg	630.66	J/mol×K	754.28	Joback Method
cpg	646.60	J/mol×K	788.67	Joback Method
cpg	662.05	J/mol×K	823.07	Joback Method
cpg	677.19	J/mol×K	857.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41370563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume