

«beta»-Copaene

Inchi: InChI=1S/C14H22/c1-8(2)10-6-7-11-12-5-4-9(3)13(11)14(10)12/h8,10-14H,3-7H2,1-2H3
InchiKey: VKJUEEOKBBSEPM-XPXVYLNCSA-N
Formula: C14H22
SMILES: C=C1CCC2C3CCC(C(C)C)C2C13
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	272.37	kJ/mol	Joback Method
hf	-81.77	kJ/mol	Joback Method
hfus	21.78	kJ/mol	Joback Method
hvap	45.82	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.881		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1441.00		NIST Webbook

rinpol	1426.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1582.00		NIST Webbook
tb	533.59	K	Joback Method
tc	741.20	K	Joback Method
tf	288.04	K	Joback Method
vc	0.658	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.39	J/molxK	533.59	Joback Method
cpg	472.90	J/molxK	568.19	Joback Method
cpg	494.02	J/molxK	602.79	Joback Method
cpg	513.84	J/molxK	637.40	Joback Method
cpg	532.46	J/molxK	672.00	Joback Method
cpg	549.94	J/molxK	706.60	Joback Method
cpg	566.37	J/molxK	741.20	Joback Method
dvisc	0.0010454	Paxs	288.04	Joback Method
dvisc	0.0011979	Paxs	328.96	Joback Method
dvisc	0.0013320	Paxs	369.89	Joback Method
dvisc	0.0014501	Paxs	410.81	Joback Method
dvisc	0.0015546	Paxs	451.74	Joback Method
dvisc	0.0016474	Paxs	492.67	Joback Method
dvisc	0.0017304	Paxs	533.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R607499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
dvisc:	Dynamic viscosity
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

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