.beta.-PANASINSENE

Inchi: InChI=1S/C15H24/c1-11-6-5-8-14(4)9-7-12-13(2,3)10-15(11,12)14/h12H,1,5-10H2,2-4H3
InchiKey: LTMKWDWWHXRNMO-UHFFFAOYSA-N
Formula: C15H24
SMILES: C=C1CCCC2(C)CCC3C(C)(C)CC132
Mol. weight [g/mol]: 204.36

Physical Properties

Property code	Value	Unit	Source
hfus	5.83	kJ/mol	Joback Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
rinpol	1413.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1413.00		NIST Webbook
ripol	1689.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.14	J/mol×K	566.57	Joback Method
cpg	522.76	J/mol×K	605.51	Joback Method
cpg	543.69	J/mol×K	644.45	Joback Method
cpg	563.39	J/mol×K	683.38	Joback Method
cpg	582.28	J/mol×K	722.32	Joback Method
cpg	600.82	J/mol×K	761.26	Joback Method
cpg	619.44	J/mol×K	800.20	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U159390&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices