«beta»-copaene

Inchi: InChI=1S/C15H24/c1-9(2)11-7-8-15(4)12-6-5-10(3)14(15)13(11)12/h9,11-14H,3,5-8H2,1-
InchiKey: UPVZPMJSRSWJHQ-UHFFFAOYSA-N
Formula: C15H24
SMILES: C=C1CCC2C3C(C(C)C)CCC2(C)C13
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hfus	18.07	kJ/mol	Joback Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
ripol	1598.00		NIST Webbook
ripol	1598.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.63	J/mol×K	556.71	Joback Method
cpg	524.39	J/mol×K	592.14	Joback Method
cpg	545.67	J/mol×K	627.57	Joback Method
cpg	565.65	J/mol×K	663.00	Joback Method
cpg	584.49	J/mol×K	698.44	Joback Method
cpg	602.37	J/mol×K	733.87	Joback Method
cpg	619.46	J/mol×K	769.30	Joback Method

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374189&Units=SI

Legend

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