

«beta»-alaskene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24/c1-11(2)14-6-5-13(4)15(14)9-7-12(3)8-10-15/h7,13H,5-6,8-10H2,1-4H

HMKLOOMRRZKSNM-DZGCQCFKSA-N

C15H24

CC1=CCC2(CC1)C(=C(C)C)CCC2C

204.35

Physical Properties

Property code	Value	Unit	Source
hfus	16.02	kJ/mol	Joback Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1520.50		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1520.50		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1738.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.06	J/mol×K	584.06	Joback Method
cpg	523.47	J/mol×K	621.92	Joback Method
cpg	544.48	J/mol×K	659.79	Joback Method
cpg	564.25	J/mol×K	697.65	Joback Method
cpg	582.97	J/mol×K	735.51	Joback Method
cpg	600.80	J/mol×K	773.38	Joback Method
cpg	617.92	J/mol×K	811.24	Joback Method

Sources

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=R190604&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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