Cyperadiene

Inchi: InChI=1S/C15H22/c1-10-7-8-15-11(2)5-6-12(9-13(10)15)14(15,3)4/h7-8,11-13H,1,5-6,9H
InchiKey: KZABVHBACHSSNR-PXWWDBQQSA-N
Formula: C15H22
SMILES: C=C1C=CC23C(C)CCC(CC12)C3(C)C
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
hfus	14.42	kJ/mol	Joback Method
logp	4.191		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
rinpol	1379.00		NIST Webbook
rinpol	1358.00		NIST Webbook
ripol	1536.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.51	J/mol×K	560.82	Joback Method
cpg	504.64	J/mol×K	598.56	Joback Method
cpg	525.18	J/mol×K	636.31	Joback Method
cpg	544.42	J/mol×K	674.05	Joback Method
cpg	562.67	J/mol×K	711.80	Joback Method
cpg	580.23	J/mol×K	749.54	Joback Method
cpg	597.39	J/mol×K	787.28	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=R428098&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices