Zonarene

Inchi: InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h9-10,12,14H,5-8H2,1-4
InchiKey: FIAKMTRUEKZMNO-TZMCWYRMSA-N
Formula: C15H24
SMILES: CC1=CC2=C(C(C)C)CCC(C)C2CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hfus	20.23	kJ/mol	Joback Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1529.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1529.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.23	J/mol×K	585.98	Joback Method
cpg	525.21	J/mol×K	622.06	Joback Method
cpg	545.92	J/mol×K	658.13	Joback Method
cpg	565.40	J/mol×K	694.21	Joback Method
cpg	583.72	J/mol×K	730.28	Joback Method
cpg	600.91	J/mol×K	766.36	Joback Method
cpg	617.03	J/mol×K	802.43	Joback Method
dvisc	0.0020981	Pa×s	304.69	Joback Method
dvisc	0.0012209	Pa×s	351.57	Joback Method
dvisc	0.0008070	Pa×s	398.45	Joback Method

dvisc	0.0005820	Pa×s	445.34	Joback Method
dvisc	0.0004467	Pa×s	492.22	Joback Method
dvisc	0.0003590	Pa×s	539.10	Joback Method
dvisc	0.0002988	Pa×s	585.98	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R609460&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):
Cheméo Relay (1.0, beta):

Legend

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