

Kessane

Inchi: InChI=1S/C15H26O/c1-10-5-6-13-12(10)9-11-7-8-15(13,4)16-14(11,2)3/h10-13H,5-9H2,1
InchiKey: QRVMFXFSGYDNJI-CEJAEVFISA-N
Formula: C15H26O
SMILES: CC1CCC2C1CC1CCC2(C)OC1(C)C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	21.31	kJ/mol	Joback Method
logp	4.016		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
rinpol	1517.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1522.70		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1530.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1786.00		NIST Webbook

ripol	1785.00	NIST Webbook
ripol	1786.00	NIST Webbook
ripol	1779.00	NIST Webbook
ripol	1786.00	NIST Webbook
ripol	1807.00	NIST Webbook
ripol	1800.00	NIST Webbook
ripol	1800.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.58	J/mol×K	589.05	Joback Method
cpg	586.42	J/mol×K	626.99	Joback Method
cpg	609.68	J/mol×K	664.93	Joback Method
cpg	631.66	J/mol×K	702.87	Joback Method
cpg	652.64	J/mol×K	740.81	Joback Method
cpg	672.91	J/mol×K	778.75	Joback Method
cpg	692.75	J/mol×K	816.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R2134&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
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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