

epi-«alpha»-Cadinol

Inchi:	InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h9-10,12-14,16H,5-
InchiKey:	LHYHMMRYTDARSZ-PPWQZUPISA-N
Formula:	C15H26O
SMILES:	CC1=CC2C(C(C)C)CCC(C)(O)C2CC1
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
hf	-285.47	kJ/mol	Cheméo Relay (1.0)
hfus	19.72	kJ/mol	Joback Method
hvap	82.40	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1639.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1634.00		NIST Webbook
tb	557.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.80	J/mol×K	659.94	Joback Method
cpg	617.79	J/mol×K	694.13	Joback Method
cpg	636.77	J/mol×K	728.33	Joback Method
cpg	654.86	J/mol×K	762.52	Joback Method

cpg	672.18	J/mol×K	796.72	Joback Method
cpg	688.83	J/mol×K	830.91	Joback Method
cpg	704.93	J/mol×K	865.11	Joback Method

Sources

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=R607088&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

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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