«delta»-Cadinol #1

Inchi: InChI=1S/C15H26O/c1-10(2)12-6-5-11(3)13-7-8-15(4,16)9-14(12)13/h5,10,12-14,16H,6-
InchiKey: ISOIDIYKQYJGMC-NAOUJUTFSA-N
Formula: C15H26O
SMILES: CC1=CCC(C(C)C)C2CC(C)(O)CCC12
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	19.72	kJ/mol	Joback Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook

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

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R83877&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

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