Cuparenal

Inchi: InChI=1S/C15H20O/c1-12-5-7-13(8-6-12)15(3)10-4-9-14(15,2)11-16/h5-8,11H,4,9-10H2,
InchiKey: LHAOCUCGEDVRKC-YSSOQSIOSA-N
Formula: C15H20O
SMILES: Cc1ccc(C2(C)CCCC2(C)C=O)cc1
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
hfus	12.96	kJ/mol	Joback Method
logp	3.642		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
rinpol	1763.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.04	J/mol×K	634.01	Joback Method
cpg	523.19	J/mol×K	674.03	Joback Method
cpg	541.31	J/mol×K	714.05	Joback Method
cpg	558.70	J/mol×K	754.07	Joback Method
cpg	575.64	J/mol×K	794.09	Joback Method
cpg	592.43	J/mol×K	834.11	Joback Method
cpg	609.38	J/mol×K	874.13	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R590559&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):

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