Vertofix coeur

Other names: Vertofix coeur
Inchi: InChI=1S/C17H26O/c1-10-6-7-15-16(4,5)14-9-17(10,15)8-13(11(14)2)12(3)18/h10,14-15
InchiKey: YBUIAJZFOGJGLJ-UHFFFAOYSA-N
Formula: C17H26O
SMILES: CC(=O)C1=C(C)C2CC3(C1)C(C)CCC3C2(C)C
Mol. weight [g/mol]: 246.39

Physical Properties

Property code	Value	Unit	Source
hfus	21.58	kJ/mol	Joback Method
logp	4.374		Crippen Method
mcvol	215.080	ml/mol	McGowan Method
rinpol	1779.80		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.03	J/mol×K	671.25	Joback Method
cpg	660.42	J/mol×K	708.74	Joback Method
cpg	680.93	J/mol×K	746.23	Joback Method
cpg	700.85	J/mol×K	783.72	Joback Method
cpg	720.46	J/mol×K	821.21	Joback Method
cpg	740.05	J/mol×K	858.71	Joback Method
cpg	759.92	J/mol×K	896.20	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68039350&Units=SI

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