Flavesone

Inchi: InChI=1S/C14H20O4/c1-7(2)9(15)8-10(16)13(3,4)12(18)14(5,6)11(8)17/h7,16H,1-6H3
InchiKey: ZOAWAFFEEBTHOX-UHFFFAOYSA-N
Formula: C14H20O4
SMILES: CC(C)C(=O)C1=C(O)C(C)(C)C(=O)C(C)(C)C1=O
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
hfus	13.95	kJ/mol	Joback Method
logp	2.228		Crippen Method
mcvol	203.540	ml/mol	McGowan Method
rinpol	1538.00		NIST Webbook
rinpol	1538.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.11	J/mol×K	825.45	Joback Method
cpg	653.33	J/mol×K	862.91	Joback Method
cpg	670.51	J/mol×K	900.38	Joback Method
cpg	687.79	J/mol×K	937.84	Joback Method
cpg	705.33	J/mol×K	975.30	Joback Method
cpg	723.27	J/mol×K	1012.77	Joback Method
cpg	741.74	J/mol×K	1050.23	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R614056&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