

(Z)-2-Methyl-6-(4-methyl-5-(3-methylbut-2-enoyl)cyclohex-1-en-1-yl)hex-3-en-2-one

Inchi: InChI=1S/C20H28O2/c1-13(2)9-18(21)11-16(6)17-8-7-15(5)19(12-17)20(22)10-14(3)4/h7-10,12-13,15-16,18-21,23-24,26-27,29-30,32-33,35-36,38-39,41-42,44-45,47-48,50-51,53-54,56-57,59-60,62-63,65-66,68-69,71-72,74-75,77-78,80-81,83-84,86-87,89-90,92-93,95-96,98-99,101-102,104-105,107-108,110-111,113-114,116-117,119-120,122-123,125-126,128-129,131-132,134-135,137-138,140-141,143-144,146-147,149-150,152-153,155-156,158-159,161-162,164-165,167-168,170-171,173-174,176-177,179-180,182-183,185-186,188-189,191-192,194-195,197-198,200-201,203-204,206-207,209-210,212-213,215-216,218-219,221-222,224-225,227-228,230-231,233-234,236-237,239-240,242-243,245-246,248-249,251-252,254-255,257-258,260-261,263-264,266-267,269-270,272-273,275-276,278-279,281-282,284-285,287-288,290-291,293-294,296-297,299-300,302-303,305-306,308-309,311-312,314-315,317-318,320-321,323-324,326-327,329-330,332-333,335-336,338-339,341-342,344-345,347-348,350-351,353-354,356-357,359-360,362-363,365-366,368-369,371-372,374-375,377-378,380-381,383-384,386-387,389-390,392-393,395-396,398-399,401-402,404-405,407-408,410-411,413-414,416-417,419-420,422-423,425-426,428-429,431-432,434-435,437-438,440-441,443-444,446-447,449-450,452-453,455-456,458-459,461-462,464-465,467-468,470-471,473-474,476-477,479-480,482-483,485-486,488-489,491-492,494-495,497-498,500-501,503-504,506-507,509-510,512-513,515-516,518-519,521-522,524-525,527-528,530-531,533-534,536-537,539-540,542-543,545-546,548-549,551-552,554-555,557-558,560-561,563-564,566-567,569-570,572-573,575-576,578-579,581-582,584-585,587-588,590-591,593-594,596-597,599-600,602-603,605-606,608-609,611-612,614-615,617-618,620-621,623-624,626-627,629-630,632-633,635-636,638-639,641-642,644-645,647-648,650-651,653-654,656-657,659-660,662-663,665-666,668-669,671-672,674-675,677-678,680-681,683-684,686-687,689-690,692-693,695-696,698-699,701-702,704-705,707-708,710-711,713-714,716-717,719-720,722-723,725-726,728-729,731-732,734-735,737-738,740-741,743-744,746-747,749-750,752-753,755-756,758-759,761-762,764-765,767-768,770-771,773-774,776-777,779-780,782-783,785-786,788-789,791-792,794-795,797-798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000

InchiKey: LASOUTDTKMMTFN-WJDWOHSUSA-N

Formula: C₂₀H₂₈O₂

SMILES: CC(C)=CC(=O)C=C(C)C1CC=C(C)C(C(=O)C=C(C)C)C1

Mol. weight [g/mol]: 300.44

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 111.76 | kJ/mol | Joback Method |
| hf | -278.71 | kJ/mol | Joback Method |
| hfus | 41.17 | kJ/mol | Joback Method |
| hvap | 74.79 | kJ/mol | Joback Method |
| log10ws | -5.58 | | Crippen Method |
| logp | 4.976 | | Crippen Method |
| mvol | 267.740 | ml/mol | McGowan Method |
| pc | 1426.15 | kPa | Joback Method |
| rinpol | 2117.50 | | NIST Webbook |
| rinpol | 2117.50 | | NIST Webbook |
| tb | 795.88 | K | Joback Method |
| tc | 1015.19 | K | Joback Method |
| tf | 374.32 | K | Joback Method |
| vc | 1.028 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 802.73 | J/molxK | 795.88 | Joback Method |
| cpg | 821.51 | J/molxK | 832.43 | Joback Method |
| cpg | 839.12 | J/molxK | 868.98 | Joback Method |
| cpg | 855.65 | J/molxK | 905.53 | Joback Method |
| cpg | 871.19 | J/molxK | 942.09 | Joback Method |
| cpg | 885.84 | J/molxK | 978.64 | Joback Method |
| cpg | 899.68 | J/molxK | 1015.19 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U414277&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

Legend

| | |
|------------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| h vap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| r in pol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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