

Glutaric acid, heptyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C17H30O5/c1-2-3-4-5-6-12-21-16(18)10-7-11-17(19)22-14-15-9-8-13-20-15/h1-17,21-22,24-25,27-28,30-31,33-34,36-37,39-40,42-43,45-46,48-49,51-52,54-55,57-58,60-61,63-64,66-67,69-70,72-73,75-76,78-79,81-82,84-85,87-88,90-91,93-94,96-97,99-100,102-103,105-106,108-109,111-112,114-115,117-118,120-121,123-124,126-127,129-130,132-133,135-136,138-139,141-142,144-145,147-148,150-151,153-154,156-157,159-160,162-163,165-166,168-169,171-172,174-175,177-178,180-181,183-184,186-187,189-190,192-193,195-196,198-199,201-202,204-205,207-208,210-211,213-214,216-217,219-220,222-223,225-226,228-229,231-232,234-235,237-238,240-241,243-244,246-247,249-250,252-253,255-256,258-259,261-262,264-265,267-268,270-271,273-274,276-277,279-280,282-283,285-286,288-289,291-292,294-295,297-298,300-301,303-304,306-307,309-310,312-313,315-316,318-319,321-322,324-325,327-328,330-331,333-334,336-337,339-340,342-343,345-346,348-349,351-352,354-355,357-358,360-361,363-364,366-367,369-370,372-373,375-376,378-379,381-382,384-385,387-388,390-391,393-394,396-397,399-400,402-403,405-406,408-409,411-412,414-415,417-418,420-421,423-424,426-427,429-430,432-433,435-436,438-439,441-442,444-445,447-448,450-451,453-454,456-457,459-460,462-463,465-466,468-469,471-472,474-475,477-478,480-481,483-484,486-487,489-490,492-493,495-496,498-499,501-502,504-505,507-508,510-511,513-514,516-517,519-520,522-523,525-526,528-529,531-532,534-535,537-538,540-541,543-544,546-547,549-550,552-553,555-556,558-559,561-562,564-565,567-568,570-571,573-574,576-577,579-580,582-583,585-586,588-589,591-592,594-595,597-598,600-601,603-604,606-607,609-610,612-613,615-616,618-619,621-622,624-625,627-628,630-631,633-634,636-637,639-640,642-643,645-646,648-649,651-652,654-655,657-658,660-661,663-664,666-667,669-670,672-673,675-676,678-679,681-682,684-685,687-688,690-691,693-694,696-697,699-700,702-703,705-706,708-709,711-712,714-715,717-718,720-721,723-724,726-727,729-730,732-733,735-736,738-739,741-742,744-745,747-748,750-751,753-754,756-757,759-760,762-763,765-766,768-769,771-772,774-775,777-778,780-781,783-784,786-787,789-790,792-793,795-796,798-799,801-802,804-805,807-808,810-811,813-814,816-817,819-820,822-823,825-826,828-829,831-832,834-835,837-838,840-841,843-844,846-847,849-850,852-853,855-856,858-859,861-862,864-865,867-868,870-871,873-874,876-877,879-880,882-883,885-886,888-889,891-892,894-895,897-898,900-901,903-904,906-907,909-910,912-913,915-916,918-919,921-922,924-925,927-928,930-931,933-934,936-937,939-940,942-943,945-946,948-949,951-952,954-955,957-958,960-961,963-964,966-967,969-970,972-973,975-976,978-979,981-982,984-985,987-988,990-991,993-994,996-997,999-1000

InchiKey: DKXPATBYXYMLAF-UHFFFAOYSA-N

Formula: C17H30O5

SMILES: CCCCCCOC(=O)CCCC(=O)OCC1CCCO1

Mol. weight [g/mol]: 314.42

Physical Properties

Property code	Value	Unit	Source
gf	-425.15	kJ/mol	Joback Method
hf	-955.33	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.393		Crippen Method
mvol	260.280	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	783.17	K	Joback Method
tc	975.39	K	Joback Method
tf	463.14	K	Joback Method
vc	0.998	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.86	J/molxK	783.17	Joback Method
cpg	893.57	J/molxK	943.35	Joback Method
cpg	880.51	J/molxK	911.32	Joback Method
cpg	866.43	J/molxK	879.28	Joback Method
cpg	851.30	J/molxK	847.24	Joback Method
cpg	835.12	J/molxK	815.21	Joback Method
cpg	905.63	J/molxK	975.39	Joback Method
dvisc	0.0001040	Paxs	783.17	Joback Method

dvisc	0.0001348	Paxs	729.83	Joback Method
dvisc	0.0001821	Paxs	676.49	Joback Method
dvisc	0.0002591	Paxs	623.15	Joback Method
dvisc	0.0003937	Paxs	569.82	Joback Method
dvisc	0.0006523	Paxs	516.48	Joback Method
dvisc	0.0012139	Paxs	463.14	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359663&Units=SI
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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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