

Diglycolic acid, 4-chlorobenzyl butyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H19ClO5/c1-2-3-8-20-14(17)10-19-11-15(18)21-9-12-4-6-13(16)7-5-12/h4-13,15-17,20-21,23-24,26-27,29-30,32-33,35-36,38-39,41-42,44-45,47-48,50-51,53-54,56-57,59-60,62-63,65-66,68-69,71-72,74-75,77-78,80-81,83-84,86-87,89-90,92-93,95-96,98-99,101-102,104-105,107-108,110-111,113-114,116-117,119-120,122-123,125-126,128-129,131-132,134-135,137-138,140-141,143-144,146-147,149-150,152-153,155-156,158-159,161-162,164-165,167-168,170-171,173-174,176-177,179-180,182-183,185-186,188-189,191-192,194-195,197-198,200-201,203-204,206-207,209-210,212-213,215-216,218-219,221-222,224-225,227-228,230-231,233-234,236-237,239-240,242-243,245-246,248-249,251-252,254-255,257-258,260-261,263-264,266-267,269-270,272-273,275-276,278-279,281-282,284-285,287-288,290-291,293-294,296-297,299-300,302-303,305-306,308-309,311-312,314-315,317-318,320-321,323-324,326-327,329-330,332-333,335-336,338-339,341-342,344-345,347-348,350-351,353-354,356-357,359-360,362-363,365-366,368-369,371-372,374-375,377-378,380-381,383-384,386-387,389-390,392-393,395-396,398-399,401-402,404-405,407-408,410-411,413-414,416-417,419-420,422-423,425-426,428-429,431-432,434-435,437-438,440-441,443-444,446-447,449-450,452-453,455-456,458-459,461-462,464-465,467-468,470-471,473-474,476-477,479-480,482-483,485-486,488-489,491-492,494-495,497-498,499-500

CGHQYYYYLFOHJOR-UHFFFAOYSA-N

C15H19ClO5

CCCCOC(=O)COCC(=O)OCc1ccc(Cl)cc1

314.76

Physical Properties

Property code	Value	Unit	Source
gf	-406.57	kJ/mol	Joback Method
hf	-765.43	kJ/mol	Joback Method
hfus	39.22	kJ/mol	Joback Method
hvap	77.03	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.743		Crippen Method
mcvol	231.440	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	2846.00		NIST Webbook
rinpol	2846.00		NIST Webbook
tb	786.69	K	Joback Method
tc	992.98	K	Joback Method
tf	494.22	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.85	J/mol×K	786.69	Joback Method
cpg	703.51	J/mol×K	958.60	Joback Method
cpg	694.17	J/mol×K	924.22	Joback Method
cpg	683.83	J/mol×K	889.84	Joback Method
cpg	672.50	J/mol×K	855.45	Joback Method
cpg	660.17	J/mol×K	821.07	Joback Method
cpg	711.86	J/mol×K	992.98	Joback Method
dvisc	0.0000717	Pa×s	786.69	Joback Method

dvisc	0.0000902	Pa×s	737.94	Joback Method
dvisc	0.0001173	Pa×s	689.20	Joback Method
dvisc	0.0001586	Pa×s	640.45	Joback Method
dvisc	0.0002255	Pa×s	591.71	Joback Method
dvisc	0.0003415	Pa×s	542.97	Joback Method
dvisc	0.0005613	Pa×s	494.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382256&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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