

Glutaric acid, 3,4-dimethylphenyl ethyl ester

Inchi:	InChI=1S/C15H20O4/c1-4-18-14(16)6-5-7-15(17)19-13-9-8-11(2)12(3)10-13/h8-10H,4-7H
InchiKey:	NXZDMVOKJCMOKV-UHFFFAOYSA-N
Formula:	C15H20O4
SMILES:	CCOC(=O)CCCC(=O)Oc1ccc(C)c(C)c1
Mol. weight [g/mol]:	264.32

Physical Properties

Property code	Value	Unit	Source
gf	-299.27	kJ/mol	Joback Method
hf	-628.94	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	70.90	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.942		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpola	2059.00		NIST Webbook
tb	731.82	K	Joback Method
tc	936.25	K	Joback Method
tf	454.59	K	Joback Method
vc	0.816	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.78	J/molxK	731.82	Joback Method
cpg	607.44	J/molxK	765.89	Joback Method
cpg	621.19	J/molxK	799.96	Joback Method
cpg	634.03	J/molxK	834.04	Joback Method
cpg	645.96	J/molxK	868.11	Joback Method
cpg	656.98	J/molxK	902.18	Joback Method
cpg	667.10	J/molxK	936.25	Joback Method
dvisc	0.0007757	Paxs	454.59	Joback Method
dvisc	0.0004776	Paxs	500.80	Joback Method

dvisc	0.0003191	Paxs	547.00	Joback Method
dvisc	0.0002270	Paxs	593.21	Joback Method
dvisc	0.0001697	Paxs	639.41	Joback Method
dvisc	0.0001319	Paxs	685.62	Joback Method
dvisc	0.0001058	Paxs	731.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359176&Units=SI

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

Latest version available from:

<https://www.chemeo.com/cid/43-299-3/Glutaric-acid-3-4-dimethylphenyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-27 07:33:12.683004664 +0000 UTC m=+16492441.603581976.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.