

Glutaric acid, (5-ethyl-1,3-dioxan-5-yl)methyl ethyl ester

Inchi:	InChI=1S/C14H24O6/c1-3-14(8-17-11-18-9-14)10-20-13(16)7-5-6-12(15)19-4-2/h3-11H2
InchiKey:	WOPHSFJGVZIHHI-UHFFFAOYSA-N
Formula:	C14H24O6
SMILES:	CCOC(=O)CCCC(=O)OCC1(CC)COCOC1
Mol. weight [g/mol]:	288.34

Physical Properties

Property code	Value	Unit	Source
gf	-554.12	kJ/mol	Joback Method
hf	-1016.33	kJ/mol	Joback Method
hfus	39.09	kJ/mol	Joback Method
hvap	73.37	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.664		Crippen Method
mcvol	223.880	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook
tb	745.99	K	Joback Method
tc	949.94	K	Joback Method
tf	476.28	K	Joback Method
vc	0.841	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.01	J/molxK	745.99	Joback Method
cpg	694.69	J/molxK	779.98	Joback Method
cpg	710.63	J/molxK	813.97	Joback Method
cpg	725.91	J/molxK	847.97	Joback Method
cpg	740.60	J/molxK	881.96	Joback Method
cpg	754.77	J/molxK	915.95	Joback Method
cpg	768.51	J/molxK	949.94	Joback Method

Sources

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=U380479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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