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

Inchi: InChI=1S/C19H32O8/c1-3-18(8-22-14-23-9-18)12-26-16(20)6-5-7-17(21)27-13-19(4-2)10

InchiKey: FXTONUMDXWNAEJ-UHFFFAOYSA-N

Formula: C19H32O8

SMILES: CCC1(COC(=O)CCCC(=O)OCC2(CC)COCOC2)COCOC1

Mol. weight [g/mol]: 388.45

Physical Properties

Property code	Value	Unit	Source
gf	-665.30	kJ/mol	Joback Method
hf	-1313.97	kJ/mol	Joback Method
hfus	53.53	kJ/mol	Joback Method
hvap	92.80	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.045		Crippen Method
mcvol	295.210	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	3153.00		NIST Webbook
rinpol	3153.00		NIST Webbook
tb	934.08	K	Joback Method
tc	1159.16	K	Joback Method
tf	617.05	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.01	J/mol×K	934.08	Joback Method
cpg	1060.46	J/mol×K	971.59	Joback Method
cpg	1082.97	J/mol×K	1009.11	Joback Method
cpg	1105.76	J/mol×K	1046.62	Joback Method
cpg	1129.05	J/mol×K	1084.13	Joback Method
cpg	1153.03	J/mol×K	1121.65	Joback Method
cpg	1177.93	J/mol×K	1159.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380498&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

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