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

Inchi: InChI=1S/C16H28O6/c1-4-16(9-19-12-20-10-16)11-22-15(18)7-5-6-14(17)21-8-13(2)3/h1

InchiKey: IMMXYWDWWCWWOV-UHFFFAOYSA-N

Formula: C16H28O6

SMILES: CCC1(COC(=O)CCCC(=O)OCC(C)C)COCOC1

Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	-539.72	kJ/mol	Joback Method
hf	-1062.89	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	77.43	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.300		Crippen Method
mcvol	252.060	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	791.31	K	Joback Method
tc	995.11	K	Joback Method
tf	483.82	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.03	J/mol×K	791.31	Joback Method
cpg	810.79	J/mol×K	825.28	Joback Method
cpg	827.78	J/mol×K	859.24	Joback Method
cpg	844.09	J/mol×K	893.21	Joback Method
cpg	859.80	J/mol×K	927.18	Joback Method
cpg	874.98	J/mol×K	961.14	Joback Method
cpg	889.72	J/mol×K	995.11	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=U380481&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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