Glutaric acid, (5-ethyl-1,3-dioxan-5-yl)methyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H34O6/c1-5-8-16(15(3)4)25-18(21)10-7-9-17(20)24-13-19(6-2)11-22-14-23

InchiKey: FBTPTZPKKGEDNM-UHFFFAOYSA-N

Formula: C19H34O6

SMILES: CCCC(OC(=O)CCCC(=O)OCC1(CC)COCOC1)C(C)C

Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-516.90	kJ/mol	Joback Method
hf	-1130.09	kJ/mol	Joback Method
hfus	44.99	kJ/mol	Joback Method
hvap	83.72	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.469		Crippen Method
mcvol	294.330	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook
tb	859.51	K	Joback Method
tc	1064.70	K	Joback Method
tf	502.63	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.97	J/mol×K	859.51	Joback Method
cpg	992.14	J/mol×K	893.71	Joback Method
cpg	1010.52	J/mol×K	927.91	Joback Method
cpg	1028.21	J/mol×K	962.10	Joback Method
cpg	1045.30	J/mol×K	996.30	Joback Method
cpg	1061.88	J/mol×K	1030.50	Joback Method
cpg	1078.05	J/mol×K	1064.70	Joback Method

Sources

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=U380484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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