Glutaric acid, 1-cyclopentylethyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C17H28O4/c1-13(2)11-12-20-16(18)9-6-10-17(19)21-14(3)15-7-4-5-8-15/h11,1

InchiKey: HBXFNNBKRQXCHB-UHFFFAOYSA-N

Formula: C17H28O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OC(C)C1CCCC1

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-269.80	kJ/mol	Joback Method
hf	-721.18	kJ/mol	Joback Method
hfus	34.66	kJ/mol	Joback Method
hvap	71.66	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.788		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	759.82	K	Joback Method
tc	961.03	K	Joback Method
tf	402.53	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.23	J/mol×K	759.82	Joback Method
cpg	777.18	J/mol×K	793.36	Joback Method
cpg	794.01	J/mol×K	826.89	Joback Method
cpg	809.75	J/mol×K	860.43	Joback Method
cpg	824.45	J/mol×K	893.96	Joback Method
cpg	838.13	J/mol×K	927.50	Joback Method
cpg	850.83	J/mol×K	961.03	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=U405460&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