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

Inchi: InChI=1S/C17H22O4/c1-13(2)10-11-20-16(18)8-5-9-17(19)21-15-7-4-6-14(3)12-15/h4,6-

InchiKey: FZLXNBGTVQHBPA-UHFFFAOYSA-N

Formula: C17H22O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1cccc(C)c1

Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-201.13	kJ/mol	Joback Method
hf	-551.32	kJ/mol	Joback Method
hfus	37.90	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.580		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
tb	776.64	K	Joback Method
tc	985.28	K	Joback Method
tf	445.57	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.98	J/mol×K	776.64	Joback Method
cpg	694.05	J/mol×K	811.41	Joback Method
cpg	708.12	J/mol×K	846.19	Joback Method
cpg	721.21	J/mol×K	880.96	Joback Method
cpg	733.34	J/mol×K	915.73	Joback Method
cpg	744.56	J/mol×K	950.50	Joback Method
cpg	754.88	J/mol×K	985.28	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=U391952&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