Glutaric acid, 3-methylbut-2-en-1-yl 4-acetylphenyl ester

Inchi: InChI=1S/C18H22O5/c1-13(2)11-12-22-17(20)5-4-6-18(21)23-16-9-7-15(8-10-16)14(3)19

InchiKey: XJXYBPFTKARXOU-UHFFFAOYSA-N

Formula: C18H22O5

SMILES: CC(=O)c1ccc(OC(=O)CCCC(=O)OCC=C(C)C)cc1

Mol. weight [g/mol]: 318.36

Physical Properties

Property code	Value	Unit	Source
gf	-321.63	kJ/mol	Joback Method
hf	-684.54	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	83.70	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.474		Crippen Method
mcvol	252.870	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	853.39	K	Joback Method
tc	1067.21	K	Joback Method
tf	506.77	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.32	J/mol×K	853.39	Joback Method
cpg	763.91	J/mol×K	889.03	Joback Method
cpg	776.45	J/mol×K	924.66	Joback Method
cpg	787.96	J/mol×K	960.30	Joback Method
cpg	798.47	J/mol×K	995.94	Joback Method
cpg	808.01	J/mol×K	1031.57	Joback Method
cpg	816.62	J/mol×K	1067.21	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392033&Units=SI

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