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

Inchi: InChI=1S/C19H26O4/c1-16(2)13-15-23-19(21)12-6-11-18(20)22-14-7-10-17-8-4-3-5-9-17

InchiKey: XDTLPXPWTZYYMK-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-174.66	kJ/mol	Joback Method
hf	-581.13	kJ/mol	Joback Method
hfus	43.47	kJ/mol	Joback Method
hvap	78.51	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.842		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook
tb	817.42	K	Joback Method
tc	1022.73	K	Joback Method
tf	455.59	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.48	J/mol×K	817.42	Joback Method
cpg	809.13	J/mol×K	851.64	Joback Method
cpg	823.73	J/mol×K	885.86	Joback Method
cpg	837.30	J/mol×K	920.08	Joback Method
cpg	849.88	J/mol×K	954.30	Joback Method
cpg	861.52	J/mol×K	988.51	Joback Method
cpg	872.25	J/mol×K	1022.73	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=U391773&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