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

Inchi: InChI=1S/C18H24O4/c1-15(2)11-13-21-17(19)9-6-10-18(20)22-14-12-16-7-4-3-5-8-16/h3

InchiKey: CZJIYNHLEVCWMH-UHFFFAOYSA-N

Formula: C18H24O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OCCc1ccccc1

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-183.08	kJ/mol	Joback Method
hf	-560.49	kJ/mol	Joback Method
hfus	40.88	kJ/mol	Joback Method
hvap	76.29	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.452		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	794.54	K	Joback Method
tc	1000.83	K	Joback Method
tf	444.32	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.20	J/mol×K	794.54	Joback Method
cpg	751.62	J/mol×K	828.92	Joback Method
cpg	766.01	J/mol×K	863.30	Joback Method
cpg	779.39	J/mol×K	897.68	Joback Method
cpg	791.80	J/mol×K	932.06	Joback Method
cpg	803.28	J/mol×K	966.44	Joback Method
cpg	813.87	J/mol×K	1000.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391789&Units=SI
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

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