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

Inchi: InChI=1S/C13H22O4/c1-10(2)8-9-16-12(14)6-5-7-13(15)17-11(3)4/h8,11H,5-7,9H2,1-4H

InchiKey: PMRZJYITKIZRAP-UHFFFAOYSA-N

Formula: C13H22O4

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

Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-340.03	kJ/mol	Joback Method
hf	-699.10	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	62.49	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.618		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	1586.00		NIST Webbook
rinpol	1586.00		NIST Webbook
tb	653.02	K	Joback Method
tc	840.60	K	Joback Method
tf	346.55	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.06	J/mol×K	653.02	Joback Method
cpg	562.14	J/mol×K	684.28	Joback Method
cpg	576.48	J/mol×K	715.55	Joback Method
cpg	590.09	J/mol×K	746.81	Joback Method
cpg	602.97	J/mol×K	778.08	Joback Method
cpg	615.14	J/mol×K	809.34	Joback Method
cpg	626.62	J/mol×K	840.60	Joback Method

Sources

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=U393371&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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