Glutaric acid, isobutyl 3-methylbut-2-enyl ester

Inchi: InChI=1S/C14H24O4/c1-11(2)8-9-17-13(15)6-5-7-14(16)18-10-12(3)4/h8,12H,5-7,9-10H2

InchiKey: KHHMNRHJPXULGG-UHFFFAOYSA-N

Formula: C14H24O4

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

Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-331.61	kJ/mol	Joback Method
hf	-719.74	kJ/mol	Joback Method
hfus	32.96	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.865		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	1765.00		NIST Webbook
tb	675.90	K	Joback Method
tc	862.07	K	Joback Method
tf	357.82	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.30	J/mol×K	675.90	Joback Method
cpg	615.87	J/mol×K	706.93	Joback Method
cpg	630.66	J/mol×K	737.96	Joback Method
cpg	644.68	J/mol×K	768.98	Joback Method
cpg	657.95	J/mol×K	800.01	Joback Method
cpg	670.48	J/mol×K	831.04	Joback Method
cpg	682.29	J/mol×K	862.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360086&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