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

Inchi: InChI=1S/C14H24O4/c1-11(2)8-9-17-13(15)6-5-7-14(16)18-10-12(3)4/h12H,1,5-10H2,2-4

InchiKey: HCEPQGMYGLGTFS-UHFFFAOYSA-N

Formula: C14H24O4

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

Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-323.99	kJ/mol	Joback Method
hf	-711.53	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	64.09	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.865		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
tb	668.42	K	Joback Method
tc	851.28	K	Joback Method
tf	361.14	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.12	J/mol×K	668.42	Joback Method
cpg	614.64	J/mol×K	698.90	Joback Method
cpg	629.40	J/mol×K	729.37	Joback Method
cpg	643.42	J/mol×K	759.85	Joback Method
cpg	656.68	J/mol×K	790.33	Joback Method
cpg	669.21	J/mol×K	820.80	Joback Method
cpg	681.01	J/mol×K	851.28	Joback Method

Sources

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=U359942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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