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

Inchi: InChI=1S/C12H20O4/c1-4-15-11(13)6-5-7-12(14)16-9-8-10(2)3/h8H,4-7,9H2,1-3H3
InchiKey: BYLBJXDKXMMJOF-UHFFFAOYSA-N
Formula: C12H20O4
SMILES: CCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 228.28

Physical Properties

Property code	Value	Unit	Source
gf	-346.01	kJ/mol	Joback Method
hf	-673.18	kJ/mol	Joback Method
hfus	31.30	kJ/mol	Joback Method
hvap	60.66	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.229		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1601.00		NIST Webbook
rinpol	1601.00		NIST Webbook
tb	630.58	K	Joback Method
tc	816.74	K	Joback Method
tf	350.28	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.77	J/mol×K	630.58	Joback Method
cpg	509.01	J/mol×K	661.61	Joback Method
cpg	522.58	J/mol×K	692.63	Joback Method
cpg	535.48	J/mol×K	723.66	Joback Method
cpg	547.73	J/mol×K	754.68	Joback Method
cpg	559.33	J/mol×K	785.71	Joback Method
cpg	570.30	J/mol×K	816.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360084&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