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

Inchi: InChI=1S/C12H20O4/c1-4-15-11(13)6-5-7-12(14)16-9-8-10(2)3/h2,4-9H2,1,3H3
InchiKey: HWRHBZZGCQLVET-UHFFFAOYSA-N
Formula: C12H20O4
SMILES: C=C(C)CCOC(=O)CCCC(=O)OCC
Mol. weight [g/mol]: 228.28

Physical Properties

Property code	Value	Unit	Source
gf	-338.39	kJ/mol	Joback Method
hf	-664.97	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.229		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	1572.00		NIST Webbook
tb	623.10	K	Joback Method
tc	805.65	K	Joback Method
tf	353.60	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.88	J/mol×K	623.10	Joback Method
cpg	508.04	J/mol×K	653.52	Joback Method
cpg	521.56	J/mol×K	683.95	Joback Method
cpg	534.43	J/mol×K	714.37	Joback Method
cpg	546.67	J/mol×K	744.80	Joback Method
cpg	558.27	J/mol×K	775.22	Joback Method
cpg	569.24	J/mol×K	805.65	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=U359940&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