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

Inchi: InChI=1S/C13H22O4/c1-4-9-16-12(14)6-5-7-13(15)17-10-8-11(2)3/h8H,4-7,9-10H2,1-3H
InchiKey: UFKHZILZARZQJF-UHFFFAOYSA-N
Formula: C13H22O4
SMILES: CCCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-337.59	kJ/mol	Joback Method
hf	-693.82	kJ/mol	Joback Method
hfus	33.89	kJ/mol	Joback Method
hvap	62.88	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.619		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	1712.00		NIST Webbook
tb	653.46	K	Joback Method
tc	838.08	K	Joback Method
tf	361.55	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.60	J/mol×K	653.46	Joback Method
cpg	561.41	J/mol×K	684.23	Joback Method
cpg	575.50	J/mol×K	715.00	Joback Method
cpg	588.90	J/mol×K	745.77	Joback Method
cpg	601.60	J/mol×K	776.54	Joback Method
cpg	613.63	J/mol×K	807.31	Joback Method
cpg	624.98	J/mol×K	838.08	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=U360085&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