Glutaric acid, 3-methylbut-2-en-1-yl 2-methylhex-3-yl ester

Inchi: InChI=1S/C17H30O4/c1-6-8-15(14(4)5)21-17(19)10-7-9-16(18)20-12-11-13(2)3/h11,14-1

InchiKey: DBEDZZZYIKVQHA-UHFFFAOYSA-N

Formula: C17H30O4

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

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-308.79	kJ/mol	Joback Method
hf	-786.94	kJ/mol	Joback Method
hfus	37.21	kJ/mol	Joback Method
hvap	71.01	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.034		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook
tb	744.10	K	Joback Method
tc	930.72	K	Joback Method
tf	376.63	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.93	J/mol×K	744.10	Joback Method
cpg	784.92	J/mol×K	775.20	Joback Method
cpg	800.99	J/mol×K	806.31	Joback Method
cpg	816.16	J/mol×K	837.41	Joback Method
cpg	830.45	J/mol×K	868.51	Joback Method
cpg	843.89	J/mol×K	899.62	Joback Method
cpg	856.48	J/mol×K	930.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393730&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