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

Inchi: InChI=1S/C18H30O4/c1-5-6-7-8-10-16(4)22-18(20)12-9-11-17(19)21-14-13-15(2)3/h8,10

InchiKey: JESDHEUYUVJEFP-CSKARUKUSA-N

Formula: C18H30O4

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

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-217.71	kJ/mol	Joback Method
hf	-685.08	kJ/mol	Joback Method
hfus	43.52	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.344		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
tb	771.58	K	Joback Method
tc	960.84	K	Joback Method
tf	397.82	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.84	J/mol×K	771.58	Joback Method
cpg	817.48	J/mol×K	803.12	Joback Method
cpg	833.21	J/mol×K	834.67	Joback Method
cpg	848.07	J/mol×K	866.21	Joback Method
cpg	862.09	J/mol×K	897.76	Joback Method
cpg	875.29	J/mol×K	929.30	Joback Method
cpg	887.72	J/mol×K	960.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393987&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