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

Inchi: InChI=1S/C18H30O4/c1-5-7-8-10-16(6-2)22-18(20)12-9-11-17(19)21-14-13-15(3)4/h6,13

InchiKey: JCSYQUGBUAKRTN-UHFFFAOYSA-N

Formula: C18H30O4

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

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-210.09	kJ/mol	Joback Method
hf	-676.87	kJ/mol	Joback Method
hfus	42.04	kJ/mol	Joback Method
hvap	72.95	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.344		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook
tb	764.10	K	Joback Method
tc	950.65	K	Joback Method
tf	401.14	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.54	J/mol×K	764.10	Joback Method
cpg	816.17	J/mol×K	795.19	Joback Method
cpg	831.90	J/mol×K	826.28	Joback Method
cpg	846.74	J/mol×K	857.38	Joback Method
cpg	860.71	J/mol×K	888.47	Joback Method
cpg	873.86	J/mol×K	919.56	Joback Method
cpg	886.19	J/mol×K	950.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405347&Units=SI

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