Glutaric acid, hexa-1,5-dien-3-yl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C16H24O4/c1-5-8-14(6-2)20-16(18)10-7-9-15(17)19-12-11-13(3)4/h5-6,11,14H

InchiKey: JSUQWQBCOJDIJD-UHFFFAOYSA-N

Formula: C16H24O4

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

Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-139.09	kJ/mol	Joback Method
hf	-510.16	kJ/mol	Joback Method
hfus	35.58	kJ/mol	Joback Method
hvap	67.83	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.340		Crippen Method
mcvol	238.280	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
rinpol	1821.00		NIST Webbook
rinpol	1821.00		NIST Webbook
tb	715.02	K	Joback Method
tc	904.00	K	Joback Method
tf	376.84	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.61	J/mol×K	715.02	Joback Method
cpg	676.98	J/mol×K	746.52	Joback Method
cpg	691.51	J/mol×K	778.01	Joback Method
cpg	705.24	J/mol×K	809.51	Joback Method
cpg	718.18	J/mol×K	841.01	Joback Method
cpg	730.37	J/mol×K	872.50	Joback Method
cpg	741.82	J/mol×K	904.00	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=U405276&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