Glutaric acid, 3-methylbut-2-en-1-yl non-5-yn-3-yl ester

Inchi: InChI=1S/C19H30O4/c1-5-7-8-9-11-17(6-2)23-19(21)13-10-12-18(20)22-15-14-16(3)4/h1
InchiKey: FXGMVWFSCMVMEF-UHFFFAOYSA-N
Formula: C19H30O4
SMILES: CCCC#CCC(CC)OC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-86.71	kJ/mol	Joback Method
hf	-550.64	kJ/mol	Joback Method
hfus	49.03	kJ/mol	Joback Method
hvap	78.00	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.181		Crippen Method
mcvol	280.550	ml/mol	McGowan Method
pc	1346.69	kPa	Joback Method
rinpol	2159.00		NIST Webbook
rinpol	2159.00		NIST Webbook
tb	799.30	K	Joback Method
tc	996.22	K	Joback Method
tf	520.27	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.34	J/mol×K	799.30	Joback Method
cpg	852.16	J/mol×K	832.12	Joback Method
cpg	867.98	J/mol×K	864.94	Joback Method
cpg	882.83	J/mol×K	897.76	Joback Method
cpg	896.74	J/mol×K	930.58	Joback Method
cpg	909.73	J/mol×K	963.40	Joback Method
cpg	921.82	J/mol×K	996.22	Joback Method

Sources

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=U393953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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