Glutaric acid, 2,6-dimethylnon-1-en-3-yn-5-yl propyl ester

Inchi: InChI=1S/C19H30O4/c1-6-9-16(5)17(13-12-15(3)4)23-19(21)11-8-10-18(20)22-14-7-2/h1

InchiKey: YZRKGDUOBYZKPB-UHFFFAOYSA-N

Formula: C19H30O4

SMILES: C=C(C)C#CC(OC(=O)CCCC(=O)OCCC)C(C)CCC

Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-81.53	kJ/mol	Joback Method
hf	-547.71	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	76.99	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.037		Crippen Method
mcvol	280.550	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	2069.00		NIST Webbook
tb	791.38	K	Joback Method
tc	987.58	K	Joback Method
tf	508.59	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.68	J/mol×K	791.38	Joback Method
cpg	851.65	J/mol×K	824.08	Joback Method
cpg	867.60	J/mol×K	856.78	Joback Method
cpg	882.54	J/mol×K	889.48	Joback Method
cpg	896.48	J/mol×K	922.18	Joback Method
cpg	909.45	J/mol×K	954.88	Joback Method
cpg	921.45	J/mol×K	987.58	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=U359818&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