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

Inchi: InChI=1S/C20H32O4/c1-6-8-15-23-19(21)11-9-12-20(22)24-18(14-13-16(3)4)17(5)10-7-2

InchiKey: AZWQOELJSPDYSC-UHFFFAOYSA-N

Formula: C20H32O4

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

Mol. weight [g/mol]: 336.47

Physical Properties

Property code	Value	Unit	Source
gf	-73.11	kJ/mol	Joback Method
hf	-568.35	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	79.21	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.428		Crippen Method
mcvol	294.640	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	814.26	K	Joback Method
tc	1010.65	K	Joback Method
tf	519.86	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.47	J/mol×K	814.26	Joback Method
cpg	910.69	J/mol×K	846.99	Joback Method
cpg	926.85	J/mol×K	879.72	Joback Method
cpg	941.96	J/mol×K	912.46	Joback Method
cpg	956.04	J/mol×K	945.19	Joback Method
cpg	969.10	J/mol×K	977.92	Joback Method
cpg	981.18	J/mol×K	1010.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359820&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