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

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

InchiKey: JYJVOFSLLWWLHJ-UHFFFAOYSA-N

Formula: C20H32O4

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

Mol. weight [g/mol]: 336.47

Physical Properties

Property code	Value	Unit	Source
gf	-75.55	kJ/mol	Joback Method
hf	-573.63	kJ/mol	Joback Method
hfus	43.09	kJ/mol	Joback Method
hvap	78.82	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.283		Crippen Method
mcvol	294.640	ml/mol	McGowan Method
pc	1261.95	kPa	Joback Method
rinpol	2121.00		NIST Webbook
tb	813.82	K	Joback Method
tc	1012.11	K	Joback Method
tf	504.86	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.97	J/mol×K	813.82	Joback Method
cpg	911.36	J/mol×K	846.87	Joback Method
cpg	927.65	J/mol×K	879.92	Joback Method
cpg	942.86	J/mol×K	912.97	Joback Method
cpg	957.01	J/mol×K	946.01	Joback Method
cpg	970.12	J/mol×K	979.06	Joback Method
cpg	982.21	J/mol×K	1012.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359819&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