Glutaric acid, 2-(adamant-1-yl)ethyl but-3-yn-2-yl ester

Inchi: InChI=1S/C21H30O4/c1-3-15(2)25-20(23)6-4-5-19(22)24-8-7-21-12-16-9-17(13-21)11-18

InchiKey: LTGWCGMAGJVFEP-UHFFFAOYSA-N

Formula: C21H30O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	35.68	kJ/mol	Joback Method
hf	-472.61	kJ/mol	Joback Method
hfus	42.25	kJ/mol	Joback Method
hvap	78.57	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.871		Crippen Method
mcvol	280.450	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	2522.00		NIST Webbook
rinpol	2522.00		NIST Webbook
tb	842.20	K	Joback Method
tc	1057.34	K	Joback Method
tf	572.68	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.42	J/mol×K	842.20	Joback Method
cpg	949.60	J/mol×K	878.06	Joback Method
cpg	969.28	J/mol×K	913.91	Joback Method
cpg	988.65	J/mol×K	949.77	Joback Method
cpg	1007.90	J/mol×K	985.63	Joback Method
cpg	1027.19	J/mol×K	1021.48	Joback Method
cpg	1046.73	J/mol×K	1057.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405376&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