Glutaric acid, 2-(adamant-1-yl)ethyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C23H34O4/c1-3-6-20(4-2)27-22(25)8-5-7-21(24)26-10-9-23-14-17-11-18(15-23

InchiKey: LQUDWJLSVQGQCZ-UHFFFAOYSA-N

Formula: C23H34O4

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

Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	32.25	kJ/mol	Joback Method
hf	-533.49	kJ/mol	Joback Method
hfus	47.58	kJ/mol	Joback Method
hvap	85.32	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.652		Crippen Method
mcvol	308.630	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2787.00		NIST Webbook
rinpol	2787.00		NIST Webbook
tb	906.84	K	Joback Method
tc	1126.95	K	Joback Method
tf	654.35	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1060.33	J/mol×K	906.84	Joback Method
cpg	1082.24	J/mol×K	943.53	Joback Method
cpg	1103.80	J/mol×K	980.21	Joback Method
cpg	1125.21	J/mol×K	1016.90	Joback Method
cpg	1146.67	J/mol×K	1053.58	Joback Method
cpg	1168.36	J/mol×K	1090.27	Joback Method
cpg	1190.48	J/mol×K	1126.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405381&Units=SI

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