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

Inchi: InChI=1S/C23H38O4/c1-4-20(16(2)3)27-22(25)7-5-6-21(24)26-9-8-23-13-17-10-18(14-23

InchiKey: FLXQYXVJFKUCED-UHFFFAOYSA-N

Formula: C23H38O4

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

Mol. weight [g/mol]: 378.55

Physical Properties

Property code	Value	Unit	Source
gf	-172.99	kJ/mol	Joback Method
hf	-811.07	kJ/mol	Joback Method
hfus	40.93	kJ/mol	Joback Method
hvap	82.78	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.284		Crippen Method
mcvol	317.230	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook
tb	897.40	K	Joback Method
tc	1108.15	K	Joback Method
tf	533.25	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1113.17	J/mol×K	897.40	Joback Method
cpg	1135.42	J/mol×K	932.53	Joback Method
cpg	1157.21	J/mol×K	967.65	Joback Method
cpg	1178.71	J/mol×K	1002.78	Joback Method
cpg	1200.10	J/mol×K	1037.90	Joback Method
cpg	1221.55	J/mol×K	1073.03	Joback Method
cpg	1243.24	J/mol×K	1108.15	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=U405378&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