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

Inchi: InChI=1S/C19H30O4/c1-2-22-17(20)4-3-5-18(21)23-7-6-19-11-14-8-15(12-19)10-16(9-14
InchiKey: NPXUJMOSPADRMB-UHFFFAOYSA-N
Formula: C19H30O4
SMILES: CCOC(=O)CCCC(=O)OCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-201.79	kJ/mol	Joback Method
hf	-717.95	kJ/mol	Joback Method
hfus	37.62	kJ/mol	Joback Method
hvap	74.65	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.870		Crippen Method
mcvol	260.870	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2405.00		NIST Webbook
rinpol	2405.00		NIST Webbook
tb	806.76	K	Joback Method
tc	1013.65	K	Joback Method
tf	518.17	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.59	J/mol×K	806.76	Joback Method
cpg	884.35	J/mol×K	841.24	Joback Method
cpg	903.47	J/mol×K	875.72	Joback Method
cpg	922.12	J/mol×K	910.20	Joback Method
cpg	940.46	J/mol×K	944.69	Joback Method
cpg	958.62	J/mol×K	979.17	Joback Method
cpg	976.77	J/mol×K	1013.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405388&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