Glutaric acid, monoamide, N-(1-adamantyl)-, isobutyl ester

Inchi: InChI=1S/C19H31NO3/c1-13(2)12-23-18(22)5-3-4-17(21)20-19-9-14-6-15(10-19)8-16(7-
InchiKey: LPGCDOFLVHWFSH-UHFFFAOYSA-N
Formula: C19H31NO3
SMILES: CC(C)COC(=O)CCCC(=O)NC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 321.45

Physical Properties

Property code	Value	Unit	Source
gf	-9.84	kJ/mol	Joback Method
hf	-537.54	kJ/mol	Joback Method
hfus	38.01	kJ/mol	Joback Method
hvap	78.29	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.441		Crippen Method
mcvol	264.980	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	2569.00		NIST Webbook
tb	834.07	K	Joback Method
tc	1045.95	K	Joback Method
tf	533.60	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.45	J/mol×K	834.07	Joback Method
cpg	917.47	J/mol×K	869.38	Joback Method
cpg	936.98	J/mol×K	904.70	Joback Method
cpg	956.16	J/mol×K	940.01	Joback Method
cpg	975.19	J/mol×K	975.32	Joback Method
cpg	994.26	J/mol×K	1010.64	Joback Method
cpg	1013.54	J/mol×K	1045.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360246&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