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

Inchi: InChI=1S/C21H35NO3/c1-15(2)5-4-8-25-20(24)7-3-6-19(23)22-21-12-16-9-17(13-21)11-

InchiKey: LATJHADXTYAOIH-UHFFFAOYSA-N

Formula: C21H35NO3

SMILES: CC(C)CCCOC(=O)CCCC(=O)NC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 349.51

Physical Properties

Property code	Value	Unit	Source
gf	7.00	kJ/mol	Joback Method
hf	-578.82	kJ/mol	Joback Method
hfus	43.19	kJ/mol	Joback Method
hvap	82.74	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.221		Crippen Method
mcvol	293.160	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpol	2774.00		NIST Webbook
tb	879.83	K	Joback Method
tc	1090.89	K	Joback Method
tf	556.14	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.63	J/mol×K	879.83	Joback Method
cpg	1041.78	J/mol×K	915.01	Joback Method
cpg	1062.56	J/mol×K	950.18	Joback Method
cpg	1083.14	J/mol×K	985.36	Joback Method
cpg	1103.70	J/mol×K	1020.54	Joback Method
cpg	1124.45	J/mol×K	1055.71	Joback Method
cpg	1145.56	J/mol×K	1090.89	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=U360249&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