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

Inchi: InChI=1S/C21H35NO3/c1-2-3-4-5-9-25-20(24)8-6-7-19(23)22-21-13-16-10-17(14-21)12-
InchiKey: ZHZDRJQXCJDYNF-UHFFFAOYSA-N
Formula: C21H35NO3
SMILES: CCCCCCOC(=O)CCCC(=O)NC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 349.51

Physical Properties

Property code	Value	Unit	Source
gf	9.44	kJ/mol	Joback Method
hf	-573.54	kJ/mol	Joback Method
hfus	46.71	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.365		Crippen Method
mcvol	293.160	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	2816.00		NIST Webbook
rinpol	2816.00		NIST Webbook
tb	880.27	K	Joback Method
tc	1089.51	K	Joback Method
tf	571.14	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.19	J/mol×K	880.27	Joback Method
cpg	1041.19	J/mol×K	915.14	Joback Method
cpg	1061.83	J/mol×K	950.02	Joback Method
cpg	1082.29	J/mol×K	984.89	Joback Method
cpg	1102.75	J/mol×K	1019.76	Joback Method
cpg	1123.39	J/mol×K	1054.64	Joback Method
cpg	1144.39	J/mol×K	1089.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360250&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

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