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

Inchi: InChI=1S/C19H31NO3/c1-2-3-7-23-18(22)6-4-5-17(21)20-19-11-14-8-15(12-19)10-16(9-
InchiKey: RPGRLTSKCSWUQH-UHFFFAOYSA-N
Formula: C19H31NO3
SMILES: CCCCOC(=O)CCCC(=O)NC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 321.45

Physical Properties

Property code	Value	Unit	Source
gf	-7.40	kJ/mol	Joback Method
hf	-532.26	kJ/mol	Joback Method
hfus	41.53	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.585		Crippen Method
mcvol	264.980	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	834.51	K	Joback Method
tc	1043.91	K	Joback Method
tf	548.60	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.97	J/mol×K	834.51	Joback Method
cpg	916.77	J/mol×K	869.41	Joback Method
cpg	936.09	J/mol×K	904.31	Joback Method
cpg	955.09	J/mol×K	939.21	Joback Method
cpg	973.96	J/mol×K	974.11	Joback Method
cpg	992.86	J/mol×K	1009.01	Joback Method
cpg	1011.98	J/mol×K	1043.91	Joback Method

Sources

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=U360247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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