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

Inchi: InChI=1S/C18H29NO3/c1-2-6-22-17(21)5-3-4-16(20)19-18-10-13-7-14(11-18)9-15(8-13)
InchiKey: VCAQEJOVOOUBDC-UHFFFAOYSA-N
Formula: C18H29NO3
SMILES: CCCOC(=O)CCCC(=O)NC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 307.43

Physical Properties

Property code	Value	Unit	Source
gf	-15.82	kJ/mol	Joback Method
hf	-511.62	kJ/mol	Joback Method
hfus	38.94	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.195		Crippen Method
mcvol	250.890	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook
tb	811.63	K	Joback Method
tc	1022.12	K	Joback Method
tf	537.33	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.91	J/mol×K	811.63	Joback Method
cpg	856.21	J/mol×K	846.71	Joback Method
cpg	874.95	J/mol×K	881.79	Joback Method
cpg	893.32	J/mol×K	916.87	Joback Method
cpg	911.49	J/mol×K	951.96	Joback Method
cpg	929.64	J/mol×K	987.04	Joback Method
cpg	947.94	J/mol×K	1022.12	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=U360245&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

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