

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

Inchi:	InChI=1S/C17H27NO3/c1-2-21-16(20)5-3-4-15(19)18-17-9-12-6-13(10-17)8-14(7-12)11-
InchiKey:	BJBSLZFHZAXNNQ-UHFFFAOYSA-N
Formula:	C17H27NO3
SMILES:	CCOC(=O)CCCC(=O)NC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	293.40

Physical Properties

Property code	Value	Unit	Source
gf	-24.24	kJ/mol	Joback Method
hf	-490.98	kJ/mol	Joback Method
hfus	36.35	kJ/mol	Joback Method
hvap	74.22	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.805		Crippen Method
mcvol	236.800	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpola	2407.00		NIST Webbook
tb	788.75	K	Joback Method
tc	1000.94	K	Joback Method
tf	526.06	K	Joback Method
vc	0.912	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.93	J/mol×K	788.75	Joback Method
cpg	796.76	J/mol×K	824.12	Joback Method
cpg	814.97	J/mol×K	859.48	Joback Method
cpg	832.75	J/mol×K	894.85	Joback Method
cpg	850.28	J/mol×K	930.21	Joback Method
cpg	867.72	J/mol×K	965.58	Joback Method
cpg	885.25	J/mol×K	1000.94	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=U360244&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
mccvol:	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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