

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

Inchi:	InChI=1S/C20H33NO3/c1-2-3-4-8-24-19(23)7-5-6-18(22)21-20-12-15-9-16(13-20)11-17(
InchiKey:	ZGJCTVYGIWOEJL-UHFFFAOYSA-N
Formula:	C20H33NO3
SMILES:	CCCCCOC(=O)CCCC(=O)NC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	335.48

Physical Properties

Property code	Value	Unit	Source
gf	1.02	kJ/mol	Joback Method
hf	-552.90	kJ/mol	Joback Method
hfus	44.12	kJ/mol	Joback Method
hvap	80.90	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	3.975		Crippen Method
mcvol	279.070	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	857.39	K	Joback Method
tc	1066.36	K	Joback Method
tf	559.87	K	Joback Method
vc	1.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.07	J/mol×K	857.39	Joback Method
cpg	978.44	J/mol×K	892.22	Joback Method
cpg	998.38	J/mol×K	927.05	Joback Method
cpg	1018.07	J/mol×K	961.87	Joback Method
cpg	1037.70	J/mol×K	996.70	Joback Method
cpg	1057.42	J/mol×K	1031.53	Joback Method
cpg	1077.44	J/mol×K	1066.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/13-924-1/Glutaric-acid-monoamide-N-1-adamantyl-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-20 03:24:08.273873318 +0000 UTC m=+15872697.194450630.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.