Aminoglutethimide

Other names:	2,6-Piperidinedione, 3-(4-aminophenyl)-3-ethyl- Glutarimide, 2-(p-aminophenyl)-2-ethyl- «alpha»-(p-Aminophenyl)-«alpha»-ethylglutarimide p-Aminoglutethimide Ba-16038 Elipten 2-(p-Aminophenyl)-2-ethylglutarimide dl-Aminoglutethimide Cytadren 3-Ethyl-3-(p-aminophenyl)-2,6-dioxopiperidine Orimeten 3-(4-Aminophenyl)-3-ethyl-2,6-piperidinedione NSC-330915
Inchi:	InChI=1S/C13H16N2O2/c1-2-13(8-7-11(16)15-12(13)17)9-3-5-10(14)6-4-9/h3-6H,2,7-8,1
InchiKey:	ROBVIMPUHSLWNV-UHFFFAOYSA-N
Formula:	C13H16N2O2
SMILES:	CCC1(c2ccc(N)cc2)CCC(=O)NC1=O
Mol. weight [g/mol]:	232.28
CAS:	125-84-8

Physical Properties

Property code	Value	Unit	Source
gf	89.30	kJ/mol	Joback Method
hf	-220.83	kJ/mol	Joback Method
hfus	22.42	kJ/mol	Joback Method
hvap	72.64	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.353		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	805.01	K	Joback Method
tc	1081.98	K	Joback Method
tf	631.22	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.77	J/mol×K	805.01	Joback Method
cpg	573.94	J/mol×K	851.17	Joback Method
cpg	591.11	J/mol×K	897.33	Joback Method
cpg	607.39	J/mol×K	943.50	Joback Method
cpg	622.92	J/mol×K	989.66	Joback Method
cpg	637.80	J/mol×K	1035.82	Joback Method
cpg	652.15	J/mol×K	1081.98	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=C125848&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