1,8-Diazacyclotetradecane-2,9-dione

Other names: 1,8-Diaza-2,9-diketocyclotetradecane
Inchi: InChI=1S/C12H22N2O2/c15-11-7-3-1-5-9-13-12(16)8-4-2-6-10-14-11/h1-10H2,(H,13,16)
InchiKey: HERSSAVMHCMYSQ-UHFFFAOYSA-N
Formula: C12H22N2O2
SMILES: O=C1CCCCCNC(=O)CCCCCN1
Mol. weight [g/mol]: 226.32
CAS: 5776-79-4

Physical Properties

Property code	Value	Unit	Source
gf	-84.24	kJ/mol	Joback Method
hf	-465.41	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	66.43	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	1.353		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
tb	765.08	K	Joback Method
tc	1052.40	K	Joback Method
tf	554.96	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.08	J/mol×K	765.08	Joback Method
cpg	626.79	J/mol×K	812.97	Joback Method
cpg	648.44	J/mol×K	860.85	Joback Method
cpg	666.79	J/mol×K	908.74	Joback Method
cpg	681.60	J/mol×K	956.63	Joback Method
cpg	692.64	J/mol×K	1004.51	Joback Method

cpg	699.67	J/mol×K	1052.40	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=C5776794&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