Cyclooctyl nitrate

Inchi: InChI=1S/C8H15NO3/c10-9(11)12-8-6-4-2-1-3-5-7-8/h8H,1-7H2
InchiKey: GERKSYFDSKVMBF-UHFFFAOYSA-N
Formula: C8H15NO3
SMILES: O=[N+]([O-])OC1CCCCCCC1
Mol. weight [g/mol]: 173.21

Physical Properties

Property code	Value	Unit	Source
gf	-52.72	kJ/mol	Joback Method
hf	-309.43	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hvap	53.18	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.308		Crippen Method
mcvol	136.010	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	1294.00		NIST Webbook
tb	584.79	K	Joback Method
tc	833.82	K	Joback Method
tf	346.10	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.00	J/mol×K	584.79	Joback Method
cpg	371.97	J/mol×K	626.29	Joback Method
cpg	389.67	J/mol×K	667.80	Joback Method
cpg	406.09	J/mol×K	709.30	Joback Method
cpg	421.24	J/mol×K	750.81	Joback Method
cpg	435.12	J/mol×K	792.31	Joback Method
cpg	447.73	J/mol×K	833.82	Joback Method

Sources

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=R497039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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