Cycloheptyl nitrate

Inchi: InChI=1S/C7H13NO3/c9-8(10)11-7-5-3-1-2-4-6-7/h7H,1-6H2
InchiKey: CAMHIRXNJVJKPY-UHFFFAOYSA-N
Formula: C7H13NO3
SMILES: O=[N+]([O-])OC1CCCCCC1
Mol. weight [g/mol]: 159.18

Physical Properties

Property code	Value	Unit	Source
gf	-49.04	kJ/mol	Joback Method
hf	-282.63	kJ/mol	Joback Method
hfus	16.17	kJ/mol	Joback Method
hvap	50.78	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	1.917		Crippen Method
mcvol	121.920	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
tb	557.64	K	Joback Method
tc	803.00	K	Joback Method
tf	338.35	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.92	J/mol×K	557.64	Joback Method
cpg	321.06	J/mol×K	598.53	Joback Method
cpg	337.10	J/mol×K	639.43	Joback Method
cpg	352.06	J/mol×K	680.32	Joback Method
cpg	365.92	J/mol×K	721.21	Joback Method
cpg	378.71	J/mol×K	762.11	Joback Method
cpg	390.42	J/mol×K	803.00	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=R496630&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