Nitric acid, hexyl ester

Other names:	n-Hexyl nitrate
	Hexyl nitrate
Inchi:	InChI=1S/C6H13NO3/c1-2-3-4-5-6-10-7(8)9/h2-6H2,1H3
InchiKey:	AGDYNDJUZRMYRG-UHFFFAOYSA-N
Formula:	C6H13NO3
SMILES:	CCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	147.17
CAS:	20633-11-8

Physical Properties

Property code	Value	Unit	Source
gf	-69.81	kJ/mol	Joback Method
hf	-310.15	kJ/mol	Joback Method
hfus	23.85	kJ/mol	Joback Method
hvap	47.95	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.775		Crippen Method
mcvol	118.690	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	1043.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1004.00		NIST Webbook
tb	510.94	K	Joback Method
tc	711.03	K	Joback Method
tf	323.22	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.96	J/mol×K	510.94	Joback Method
cpg	284.51	J/mol×K	544.29	Joback Method
cpg	295.54	J/mol×K	577.64	Joback Method
cpg	306.07	J/mol×K	610.99	Joback Method

cpg	316.10	J/mol×K	644.34	Joback Method
cpg	325.64	J/mol×K	677.69	Joback Method
cpg	334.70	J/mol×K	711.03	Joback Method

Sources

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=C20633118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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