

Nitric acid, heptyl ester

Other names:	n-Heptyl nitrate Heptyl nitrate
Inchi:	InChI=1S/C7H15NO3/c1-2-3-4-5-6-7-11-8(9)10/h2-7H2,1H3
InchiKey:	JYMDZTRYDIQILZ-UHFFFAOYSA-N
Formula:	C7H15NO3
SMILES:	CCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	161.20
CAS:	20633-12-9

Physical Properties

Property code	Value	Unit	Source
gf	-61.39	kJ/mol	Joback Method
hf	-330.79	kJ/mol	Joback Method
hfus	26.43	kJ/mol	Joback Method
hvap	50.18	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.165		Crippen Method
mcvol	132.780	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
tb	533.82	K	Joback Method
tc	731.18	K	Joback Method
tf	334.49	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.05	J/molxK	533.82	Joback Method
cpg	329.60	J/molxK	566.71	Joback Method
cpg	341.59	J/molxK	599.61	Joback Method
cpg	353.03	J/molxK	632.50	Joback Method

cpg	363.91	J/mol×K	665.40	Joback Method
cpg	374.25	J/mol×K	698.29	Joback Method
cpg	384.06	J/mol×K	731.18	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=C20633129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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

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