2-Heptyl nitrate

Inchi: InChI=1S/C7H15NO3/c1-3-4-5-6-7(2)11-8(9)10/h7H,3-6H2,1-2H3
InchiKey: HHXLSUKHLTZWKR-UHFFFAOYSA-N
Formula: C7H15NO3
SMILES: CCCCCC(C)O[N+](=O)[O-]
Mol. weight [g/mol]: 161.20

Physical Properties

Property code	Value	Unit	Source
gf	-63.83	kJ/mol	Joback Method
hf	-336.07	kJ/mol	Joback Method
hfus	22.91	kJ/mol	Joback Method
hvap	49.79	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.163		Crippen Method
mcvol	132.780	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1049.00		NIST Webbook
tb	533.38	K	Joback Method
tc	734.96	K	Joback Method
tf	319.49	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.37	J/mol×K	533.38	Joback Method
cpg	330.26	J/mol×K	566.98	Joback Method
cpg	342.55	J/mol×K	600.57	Joback Method
cpg	354.25	J/mol×K	634.17	Joback Method
cpg	365.37	J/mol×K	667.77	Joback Method
cpg	375.91	J/mol×K	701.37	Joback Method
cpg	385.89	J/mol×K	734.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496754&Units=SI
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

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