Nitric acid, decyl ester

Other names:	Decyl nitrate
	n-Decyl nitrate
Inchi:	InChI=1S/C10H21NO3/c1-2-3-4-5-6-7-8-9-10-14-11(12)13/h2-10H2,1H3
InchiKey:	UEFBRXQBUTYIJI-UHFFFAOYSA-N
Formula:	C10H21NO3
SMILES:	CCCCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	203.28
CAS:	2050-78-4

Physical Properties

Property code	Value	Unit	Source
gf	-36.13	kJ/mol	Joback Method
hf	-392.71	kJ/mol	Joback Method
hfus	34.20	kJ/mol	Joback Method
hvap	56.86	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.335		Crippen Method
mcvol	175.050	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1411.00		NIST Webbook
tb	602.46	K	Joback Method
tc	792.44	K	Joback Method
tf	368.30	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.15	J/mol×K	602.46	Joback Method
cpg	475.05	J/mol×K	634.12	Joback Method
cpg	489.25	J/mol×K	665.79	Joback Method
cpg	502.76	J/mol×K	697.45	Joback Method
cpg	515.60	J/mol×K	729.11	Joback Method
cpg	527.79	J/mol×K	760.78	Joback Method

cpg	539.32	J/mol×K	792.44	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31457e+01
Coeff. B	-3.79120e+03
Coeff. C	-8.01500e+01
Temperature range (K), min.	375.00
Temperature range (K), max.	564.08

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050784&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap: Vapor pressure
rinpol: Non-polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume