Nitric acid, 2-methylpropyl ester

Other names: ?
Isobutyl nitrate
Nitric acid, isobutyl ester
Inchi: InChI=1S/C4H9NO3/c1-4(2)3-8-5(6)7/h4H,3H2,1-2H3
InchiKey: LNNXFUZKZLXPOF-UHFFFAOYSA-N
Formula: C4H9NO3
SMILES: CC(C)CO[N+](=O)[O-]
Mol. weight [g/mol]: 119.12
CAS: 543-29-3

Physical Properties

Property code	Value	Unit	Source
gf	-89.09	kJ/mol	Joback Method
hf	-274.15	kJ/mol	Joback Method
hfus	15.14	kJ/mol	Joback Method
hvap	42.17	kJ/mol	NIST Webbook
log10ws	-1.42		Crippen Method
logp	0.851		Crippen Method
mcvol	90.510	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
rinpol	739.00		NIST Webbook
tb	396.60	K	NIST Webbook
tb	396.75 ± 0.40	K	NIST Webbook
tb	396.05 ± 0.30	K	NIST Webbook
tb	397.15 ± 2.00	K	NIST Webbook
tc	675.22	K	Joback Method
tf	285.68	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.06	J/mol×K	640.14	Joback Method
cpg	191.08	J/mol×K	464.74	Joback Method

cpg	200.48	J/mol×K	499.82	Joback Method
cpg	209.47	J/mol×K	534.90	Joback Method
cpg	218.07	J/mol×K	569.98	Joback Method
cpg	226.27	J/mol×K	605.06	Joback Method
cpg	241.46	J/mol×K	675.22	Joback Method
hvapt	42.80	kJ/mol	308.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46131e+01
Coeff. B	-3.45028e+03
Coeff. C	-5.13910e+01
Temperature range (K), min.	292.24
Temperature range (K), max.	422.32

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C543293&Units=SI

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

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

hvapt: Enthalpy of vaporization at a given temperature

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