2-Methyl-3-butyl nitrate

Inchi: InChI=1S/C5H11NO3/c1-4(2)5(3)9-6(7)8/h4-5H,1-3H3
InchiKey: OTVLXFGCWJFXJU-UHFFFAOYSA-N
Formula: C5H11NO3
SMILES: CC(C)C(C)O[N+](=O)[O-]
Mol. weight [g/mol]: 133.15

Physical Properties

Property code	Value	Unit	Source
gf	-83.11	kJ/mol	Joback Method
hf	-300.07	kJ/mol	Joback Method
hfus	14.21	kJ/mol	Joback Method
hvap	44.95	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.239		Crippen Method
mcvol	104.600	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
rinpol	819.00		NIST Webbook
rinpol	819.00		NIST Webbook
tb	487.18	K	Joback Method
tc	699.50	K	Joback Method
tf	281.95	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.36	J/mol×K	487.18	Joback Method
cpg	242.40	J/mol×K	522.57	Joback Method
cpg	252.94	J/mol×K	557.95	Joback Method
cpg	262.97	J/mol×K	593.34	Joback Method
cpg	272.50	J/mol×K	628.73	Joback Method
cpg	281.53	J/mol×K	664.12	Joback Method
cpg	290.07	J/mol×K	699.50	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=R496789&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