2,2-Dimethyl-3-butyl nitrate

Inchi: InChI=1S/C6H13NO3/c1-5(6(2,3)4)10-7(8)9/h5H,1-4H3
InchiKey: YUZOHIKIQPTSGJ-UHFFFAOYSA-N
Formula: C6H13NO3
SMILES: CC(O[N+](=O)[O-])C(C)(C)C
Mol. weight [g/mol]: 147.17

Physical Properties

Property code	Value	Unit	Source
gf	-69.41	kJ/mol	Joback Method
hf	-324.18	kJ/mol	Joback Method
hfus	12.91	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.629		Crippen Method
mcvol	118.690	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	873.00		NIST Webbook
rinpol	873.00		NIST Webbook
tb	507.27	K	Joback Method
tc	725.19	K	Joback Method
tf	310.64	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.63	J/mol×K	507.27	Joback Method
cpg	289.50	J/mol×K	543.59	Joback Method
cpg	301.60	J/mol×K	579.91	Joback Method
cpg	312.97	J/mol×K	616.23	Joback Method
cpg	323.64	J/mol×K	652.55	Joback Method
cpg	333.64	J/mol×K	688.87	Joback Method
cpg	342.99	J/mol×K	725.19	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=R496714&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