2,4-Dimethyl-4-heptyl nitrate

Inchi: InChI=1S/C9H19NO3/c1-5-6-9(4,7-8(2)3)13-10(11)12/h8H,5-7H2,1-4H3
InchiKey: GJFSGBJZEYDMKR-UHFFFAOYSA-N
Formula: C9H19NO3
SMILES: CCCC(C)(CC(C)C)O[N+](=O)[O-]
Mol. weight [g/mol]: 189.25

Physical Properties

Property code	Value	Unit	Source
gf	-44.15	kJ/mol	Joback Method
hf	-386.10	kJ/mol	Joback Method
hfus	20.68	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.800		Crippen Method
mcvol	160.960	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1119.00		NIST Webbook
tb	575.91	K	Joback Method
tc	783.42	K	Joback Method
tf	344.45	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.40	J/mol×K	575.91	Joback Method
cpg	429.79	J/mol×K	610.49	Joback Method
cpg	444.30	J/mol×K	645.08	Joback Method
cpg	457.97	J/mol×K	679.66	Joback Method
cpg	470.82	J/mol×K	714.25	Joback Method
cpg	482.91	J/mol×K	748.83	Joback Method
cpg	494.24	J/mol×K	783.42	Joback Method

Sources

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=R496729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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