Pentane, 2,2,4-trimethyl-4-nitro-

Other names:	2-Nitro-2,4,4-trimethylpentane
	2,4,4-Trimethyl-2-nitropentane
Inchi:	InChI=1S/C8H17NO2/c1-7(2,3)6-8(4,5)9(10)11/h6H2,1-5H3
InchiKey:	CUEFTLGHWYSCTO-UHFFFAOYSA-N
Formula:	C8H17NO2
SMILES:	CC(C)(C)CC(C)(C)[N+](=O)[O-]
Mol. weight [g/mol]:	159.23
CAS:	5342-78-9

Physical Properties

Property code	Value	Unit	Source
gf	57.71	kJ/mol	Joback Method
hf	-236.71	kJ/mol	Joback Method
hfus	13.01	kJ/mol	Joback Method
hvap	54.70 ± 0.80	kJ/mol	NIST Webbook
log10ws	-3.13		Crippen Method
logp	2.478		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	527.82	K	Joback Method
tc	749.84	K	Joback Method
tf	296.75 ± 0.50	K	NIST Webbook
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.08	J/mol×K	712.84	Joback Method
cpg	344.84	J/mol×K	527.82	Joback Method
cpg	360.60	J/mol×K	564.82	Joback Method
cpg	375.23	J/mol×K	601.83	Joback Method
cpg	388.80	J/mol×K	638.83	Joback Method
cpg	401.40	J/mol×K	675.83	Joback Method
cpg	423.93	J/mol×K	749.84	Joback Method

hvapt	54.20 ± 0.80	kJ/mol	306.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5342789&Units=SI
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

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