O-nitro carbanilic acid, tetrahydrolinalyl ester

Inchi: InChI=1S/C17H26N2O4/c1-5-17(4,12-8-9-13(2)3)23-16(20)18-14-10-6-7-11-15(14)19(21
InchiKey: GAJANIKNWMGRMU-UHFFFAOYSA-N
Formula: C17H26N2O4
SMILES: CCC(C)(CCCC(C)C)OC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 322.40
CAS: 93814-56-3

Physical Properties

Property code	Value	Unit	Source
gf	86.46	kJ/mol	Joback Method
hf	-385.27	kJ/mol	Joback Method
hfus	41.75	kJ/mol	Joback Method
hvap	86.87	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.138		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
tb	894.65	K	Joback Method
tc	1121.45	K	Joback Method
tf	576.14	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.62	J/mol×K	894.65	Joback Method
cpg	844.83	J/mol×K	932.45	Joback Method
cpg	857.91	J/mol×K	970.25	Joback Method
cpg	869.93	J/mol×K	1008.05	Joback Method
cpg	880.97	J/mol×K	1045.85	Joback Method
cpg	891.10	J/mol×K	1083.65	Joback Method
cpg	900.41	J/mol×K	1121.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93814563&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
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