M-nitro carbanilic acid, n-pentyl ester

Inchi: InChI=1S/C12H16N2O4/c1-2-3-4-8-18-12(15)13-10-6-5-7-11(9-10)14(16)17/h5-7,9H,2-4
InchiKey: RTPZTRBFYLRPGI-UHFFFAOYSA-N
Formula: C12H16N2O4
SMILES: CCCCCOC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 252.27
CAS: 92848-37-8

Physical Properties

Property code	Value	Unit	Source
gf	43.96	kJ/mol	Joback Method
hf	-268.04	kJ/mol	Joback Method
hfus	39.73	kJ/mol	Joback Method
hvap	77.43	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.333		Crippen Method
mcvol	191.020	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
tb	783.92	K	Joback Method
tc	1010.94	K	Joback Method
tf	532.37	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.49	J/mol×K	783.92	Joback Method
cpg	561.07	J/mol×K	821.76	Joback Method
cpg	572.65	J/mol×K	859.59	Joback Method
cpg	583.28	J/mol×K	897.43	Joback Method
cpg	592.97	J/mol×K	935.27	Joback Method
cpg	601.77	J/mol×K	973.11	Joback Method
cpg	609.70	J/mol×K	1010.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92848378&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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