Alpha-(2,4-dinitrophenylamino) adipic acid

Inchi: InChI=1S/C12H13N3O8/c16-11(17)3-1-2-9(12(18)19)13-8-5-4-7(14(20)21)6-10(8)15(22)
InchiKey: PQJNHNKWSGOOGA-UHFFFAOYSA-N
Formula: C12H13N3O8
SMILES: O=C(O)CCCC(Nc1ccc([N+](=O)[O-])cc1[N+](=O)[O-])C(=O)O
Mol. weight [g/mol]: 327.25
CAS: 91719-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-230.12	kJ/mol	Joback Method
hf	-580.37	kJ/mol	Joback Method
hfus	55.77	kJ/mol	Joback Method
hvap	131.99	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	1.623		Crippen Method
mcvol	215.880	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	1156.11	K	Joback Method
tc	1415.40	K	Joback Method
tf	822.84	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.66	J/mol×K	1156.11	Joback Method
cpg	688.51	J/mol×K	1199.33	Joback Method
cpg	692.66	J/mol×K	1242.54	Joback Method
cpg	696.19	J/mol×K	1285.76	Joback Method
cpg	699.16	J/mol×K	1328.97	Joback Method
cpg	701.66	J/mol×K	1372.19	Joback Method
cpg	703.77	J/mol×K	1415.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91719594&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