2,2'-Dinitro-4,4'-biacetanilide

Inchi: InChI=1S/C16H14N4O6/c1-9(21)17-13-5-3-11(7-15(13)19(23)24)12-4-6-14(18-10(2)22)1
InchiKey: VGFDUXNDMUMYHD-UHFFFAOYSA-N
Formula: C16H14N4O6
SMILES: CC(=O)Nc1ccc(-c2ccc(NC(C)=O)c([N+](=O)[O-])c2)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 358.31
CAS: 6378-90-1

Physical Properties

Property code	Value	Unit	Source
gf	262.18	kJ/mol	Joback Method
hf	-86.13	kJ/mol	Joback Method
hfus	59.84	kJ/mol	Joback Method
hvap	117.96	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	3.087		Crippen Method
mcvol	246.720	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
tb	1150.52	K	Joback Method
tc	1424.94	K	Joback Method
tf	865.40	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.05	J/mol×K	1150.52	Joback Method
cpg	772.81	J/mol×K	1196.26	Joback Method
cpg	777.59	J/mol×K	1241.99	Joback Method
cpg	781.48	J/mol×K	1287.73	Joback Method
cpg	784.59	J/mol×K	1333.47	Joback Method
cpg	787.00	J/mol×K	1379.20	Joback Method
cpg	788.82	J/mol×K	1424.94	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=C6378901&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume