Acetamide, n-(3,7-dinitro-9-oxofluoren-2-yl)-

Inchi: InChI=1S/C15H9N3O6/c1-7(19)16-13-5-12-10(6-14(13)18(23)24)9-3-2-8(17(21)22)4-11(
InchiKey: AAGDPOKIFBYAMI-UHFFFAOYSA-N
Formula: C15H9N3O6
SMILES: CC(=O)Nc1cc2c(cc1[N+](=O)[O-])-c1ccc([N+](=O)[O-])cc1C2=O
Mol. weight [g/mol]: 327.25
CAS: 100964-96-3

Physical Properties

Property code	Value	Unit	Source
gf	253.73	kJ/mol	Joback Method
hf	-50.09	kJ/mol	Joback Method
hfus	50.94	kJ/mol	Joback Method
hvap	107.33	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	2.673		Crippen Method
mcvol	211.790	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	1099.27	K	Joback Method
tc	1380.87	K	Joback Method
tf	861.50	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.53	J/mol×K	1099.27	Joback Method
cpg	655.74	J/mol×K	1146.20	Joback Method
cpg	663.46	J/mol×K	1193.14	Joback Method
cpg	670.82	J/mol×K	1240.07	Joback Method
cpg	677.95	J/mol×K	1287.00	Joback Method
cpg	684.98	J/mol×K	1333.94	Joback Method
cpg	692.04	J/mol×K	1380.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100964963&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