Fluoranthene, 2,7-dinitro

Inchi: InChI=1S/C16H8N2O4/c19-17(20)10-7-9-3-1-5-12-15(9)13(8-10)11-4-2-6-14(16(11)12)18
InchiKey: AGIQTABGQSEBNX-UHFFFAOYSA-N
Formula: C16H8N2O4
SMILES: O=[N+]([O-])c1cc2c3c(cccc3c1)-c1c-2cccc1[N+](=O)[O-]
Mol. weight [g/mol]: 292.25

Physical Properties

Property code	Value	Unit	Source
gf	543.02	kJ/mol	Joback Method
hf	323.31	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	93.60	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	4.304		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	472.50		NIST Webbook
rinpol	472.50		NIST Webbook
tb	965.00	K	Joback Method
tc	1252.37	K	Joback Method
tf	738.18	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.72	J/mol×K	965.00	Joback Method
cpg	565.01	J/mol×K	1012.90	Joback Method
cpg	576.59	J/mol×K	1060.79	Joback Method
cpg	588.77	J/mol×K	1108.69	Joback Method
cpg	601.84	J/mol×K	1156.58	Joback Method
cpg	616.09	J/mol×K	1204.48	Joback Method
cpg	631.81	J/mol×K	1252.37	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=R36953&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume