3,4-Di-p-nitro-benzoyl-heptane

Inchi: InChI=1S/C21H22N2O6/c1-3-5-19(21(25)15-8-12-17(13-9-15)23(28)29)18(4-2)20(24)14-
InchiKey: MDLFKHBGARTENC-UHFFFAOYSA-N
Formula: C21H22N2O6
SMILES: CCCC(C(=O)c1ccc([N+](=O)[O-])cc1)C(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 398.41
CAS: 116435-50-8

Physical Properties

Property code	Value	Unit	Source
gf	139.88	kJ/mol	Joback Method
hf	-283.89	kJ/mol	Joback Method
hfus	56.32	kJ/mol	Joback Method
hvap	114.11	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	5.011		Crippen Method
mcvol	297.210	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
tb	1153.74	K	Joback Method
tc	1423.27	K	Joback Method
tf	761.39	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.90	J/mol×K	1153.74	Joback Method
cpg	979.83	J/mol×K	1198.66	Joback Method
cpg	987.81	J/mol×K	1243.58	Joback Method
cpg	994.98	J/mol×K	1288.50	Joback Method
cpg	1001.47	J/mol×K	1333.42	Joback Method
cpg	1007.44	J/mol×K	1378.35	Joback Method
cpg	1013.02	J/mol×K	1423.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116435508&Units=SI

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