10-Chlorodecyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C17H23ClN2O6/c18-9-7-5-3-1-2-4-6-8-10-26-17(21)14-11-15(19(22)23)13-16(
InchiKey: STQBXYQWLKKLHF-UHFFFAOYSA-N
Formula: C17H23ClN2O6
SMILES: O=C(OCCCCCCCCCCCCl)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 386.83

Physical Properties

Property code	Value	Unit	Source
gf	10.66	kJ/mol	Joback Method
hf	-462.68	kJ/mol	Joback Method
hfus	62.76	kJ/mol	Joback Method
hvap	103.76	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	5.019		Crippen Method
mcvol	281.150	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	2988.00		NIST Webbook
rinpol	2988.00		NIST Webbook
tb	1042.40	K	Joback Method
tc	1284.64	K	Joback Method
tf	722.11	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.99	J/mol×K	1042.40	Joback Method
cpg	902.15	J/mol×K	1082.77	Joback Method
cpg	911.15	J/mol×K	1123.15	Joback Method
cpg	919.07	J/mol×K	1163.52	Joback Method
cpg	925.95	J/mol×K	1203.89	Joback Method
cpg	931.86	J/mol×K	1244.27	Joback Method
cpg	936.85	J/mol×K	1284.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373869&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume