undecyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C18H26N2O6/c1-2-3-4-5-6-7-8-9-10-11-26-18(21)15-12-16(19(22)23)14-17(13
InchiKey: SBXUHPSCAVGZDS-UHFFFAOYSA-N
Formula: C18H26N2O6
SMILES: CCCCCCCCCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 366.41

Physical Properties

Property code	Value	Unit	Source
gf	31.01	kJ/mol	Joback Method
hf	-467.58	kJ/mol	Joback Method
hfus	61.15	kJ/mol	Joback Method
hvap	101.60	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	5.191		Crippen Method
mcvol	283.000	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2663.00		NIST Webbook
rinpol	2677.00		NIST Webbook
rinpol	2651.00		NIST Webbook
rinpol	2651.00		NIST Webbook
rinpol	2686.00		NIST Webbook
ripol	3605.00		NIST Webbook
ripol	3589.00		NIST Webbook
ripol	3616.00		NIST Webbook
tb	1027.85	K	Joback Method
tc	1265.91	K	Joback Method
tf	703.46	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.14	J/mol×K	1027.85	Joback Method
cpg	943.61	J/mol×K	1067.53	Joback Method

cpg	953.86	J/mol×K	1107.20	Joback Method
cpg	962.96	J/mol×K	1146.88	Joback Method
cpg	970.97	J/mol×K	1186.55	Joback Method
cpg	977.93	J/mol×K	1226.23	Joback Method
cpg	983.92	J/mol×K	1265.91	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=R312399&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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