decyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C17H24N2O6/c1-2-3-4-5-6-7-8-9-10-25-17(20)14-11-15(18(21)22)13-16(12-14
InchiKey: KFSXELPKFVNIRV-UHFFFAOYSA-N
Formula: C17H24N2O6
SMILES: CCCCCCCCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 352.38

Physical Properties

Property code	Value	Unit	Source
gf	22.59	kJ/mol	Joback Method
hf	-446.94	kJ/mol	Joback Method
hfus	58.56	kJ/mol	Joback Method
hvap	99.37	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	4.800		Crippen Method
mcvol	268.910	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2581.00		NIST Webbook
rinpol	2578.00		NIST Webbook
rinpol	2564.00		NIST Webbook
rinpol	2541.00		NIST Webbook
rinpol	2541.00		NIST Webbook
rinpol	2552.00		NIST Webbook
ripol	3505.00		NIST Webbook
ripol	3515.00		NIST Webbook
ripol	3469.00		NIST Webbook
ripol	3469.00		NIST Webbook
ripol	3490.00		NIST Webbook
tb	1004.97	K	Joback Method
tc	1242.30	K	Joback Method
tf	692.19	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.26	J/mol×K	1004.97	Joback Method
cpg	884.58	J/mol×K	1044.53	Joback Method
cpg	894.73	J/mol×K	1084.08	Joback Method
cpg	903.73	J/mol×K	1123.64	Joback Method
cpg	911.67	J/mol×K	1163.19	Joback Method
cpg	918.57	J/mol×K	1202.75	Joback Method
cpg	924.50	J/mol×K	1242.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312364&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
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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