

nonyl 3,5-dinitrobenzoate

Inchi:	InChI=1S/C16H22N2O6/c1-2-3-4-5-6-7-8-9-24-16(19)13-10-14(17(20)21)12-15(11-13)18
InchiKey:	MTOOOFSAJJQHCZ-UHFFFAOYSA-N
Formula:	C16H22N2O6
SMILES:	CCCCCCCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	338.36

Physical Properties

Property code	Value	Unit	Source
gf	14.17	kJ/mol	Joback Method
hf	-426.30	kJ/mol	Joback Method
hfus	55.97	kJ/mol	Joback Method
hvap	97.15	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.410		Crippen Method
mcvol	254.820	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2442.00		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	2442.00		NIST Webbook
rinpol	2478.00		NIST Webbook
rinpol	2467.00		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	2454.00		NIST Webbook
ripol	3413.00		NIST Webbook
ripol	3406.00		NIST Webbook
ripol	3413.00		NIST Webbook
ripol	3367.00		NIST Webbook
ripol	3367.00		NIST Webbook
ripol	3390.00		NIST Webbook
tb	982.09	K	Joback Method
tc	1219.61	K	Joback Method
tf	680.92	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.95	J/mol×K	982.09	Joback Method
cpg	826.13	J/mol×K	1021.68	Joback Method
cpg	836.15	J/mol×K	1061.26	Joback Method
cpg	845.06	J/mol×K	1100.85	Joback Method
cpg	852.90	J/mol×K	1140.44	Joback Method
cpg	859.73	J/mol×K	1180.02	Joback Method
cpg	865.59	J/mol×K	1219.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R312384&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
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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