

Pent-4-enyl 3,5-dinitrobenzoate

Other names:	Benzoic acid, 3,5-dinitro, 4-pentenyl ester 4-Pentenyl 3,5-dinitrobenzoate
Inchi:	InChI=1S/C12H12N2O6/c1-2-3-4-5-20-12(15)9-6-10(13(16)17)8-11(7-9)14(18)19/h2,6-8
InchiKey:	NRLCGTBUQXDVDM-UHFFFAOYSA-N
Formula:	C12H12N2O6
SMILES:	C=CCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	280.23

Physical Properties

Property code	Value	Unit	Source
gf	68.33	kJ/mol	Joback Method
hf	-218.31	kJ/mol	Joback Method
hfus	44.33	kJ/mol	Joback Method
hvap	87.57	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	2.626		Crippen Method
mcvol	194.160	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2049.00		NIST Webbook
ripol	3060.00		NIST Webbook
ripol	3085.00		NIST Webbook
ripol	3073.00		NIST Webbook
ripol	3042.00		NIST Webbook
tb	887.25	K	Joback Method
tc	1137.53	K	Joback Method
tf	634.08	K	Joback Method
vc	0.768	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	561.06	J/mol×K	887.25	Joback Method
cpg	570.89	J/mol×K	928.96	Joback Method
cpg	579.69	J/mol×K	970.68	Joback Method
cpg	587.50	J/mol×K	1012.39	Joback Method
cpg	594.37	J/mol×K	1054.10	Joback Method
cpg	600.34	J/mol×K	1095.82	Joback Method
cpg	605.46	J/mol×K	1137.53	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=U373865&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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