Benzoic acid, 3,5-dinitro, allyl ester

Other names: 2-Propenyl 3,5-dinitrobenzoate
Inchi: InChI=1S/C10H8N2O6/c1-2-3-18-10(13)7-4-8(11(14)15)6-9(5-7)12(16)17/h2,4-6H,1,3H2
InchiKey: HUQSUNYFBNIPTL-UHFFFAOYSA-N
Formula: C10H8N2O6
SMILES: C=CCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 252.18

Physical Properties

Property code	Value	Unit	Source
gf	51.49	kJ/mol	Joback Method
hf	-177.03	kJ/mol	Joback Method
hfus	39.15	kJ/mol	Joback Method
hvap	83.12	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	1.846		Crippen Method
mcvol	165.980	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1833.00		NIST Webbook
ripol	2879.00		NIST Webbook
ripol	2880.00		NIST Webbook
ripol	2863.00		NIST Webbook
ripol	2900.00		NIST Webbook
ripol	2880.00		NIST Webbook
tb	841.49	K	Joback Method
tc	1101.36	K	Joback Method
tf	611.54	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	453.84	J/mol×K	841.49	Joback Method
cpg	462.85	J/mol×K	884.80	Joback Method
cpg	470.87	J/mol×K	928.11	Joback Method
cpg	477.94	J/mol×K	971.43	Joback Method
cpg	484.09	J/mol×K	1014.74	Joback Method
cpg	489.37	J/mol×K	1058.05	Joback Method
cpg	493.81	J/mol×K	1101.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R34650&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume