Benzoic acid, 4-nitro, 1,2-dimethylpropyl ester

Inchi: InChI=1S/C12H15NO4/c1-8(2)9(3)17-12(14)10-4-6-11(7-5-10)13(15)16/h4-9H,1-3H3
InchiKey: LYLZAGFMDOUGKM-UHFFFAOYSA-N
Formula: C12H15NO4
SMILES: CC(C)C(C)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 237.25

Physical Properties

Property code	Value	Unit	Source
gf	-50.31	kJ/mol	Joback Method
hf	-332.07	kJ/mol	Joback Method
hfus	27.59	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.796		Crippen Method
mcvol	181.040	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1710.00		NIST Webbook
ripol	2425.00		NIST Webbook
ripol	2465.00		NIST Webbook
ripol	2413.00		NIST Webbook
ripol	2425.00		NIST Webbook
ripol	2440.00		NIST Webbook
tb	732.87	K	Joback Method
tc	969.98	K	Joback Method
tf	449.71	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.70	J/mol×K	732.87	Joback Method

cpg	512.46	J/mol×K	772.39	Joback Method
cpg	525.14	J/mol×K	811.91	Joback Method
cpg	536.78	J/mol×K	851.43	Joback Method
cpg	547.39	J/mol×K	890.94	Joback Method
cpg	557.03	J/mol×K	930.46	Joback Method
cpg	565.70	J/mol×K	969.98	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=R35335&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