Fumaric acid, isobutyl 3-nitrophenyl ester

Inchi: InChI=1S/C14H15NO6/c1-10(2)9-20-13(16)6-7-14(17)21-12-5-3-4-11(8-12)15(18)19/h3-8
InchiKey: ASMQUBPIPQANDH-VOTSOKGWSA-N
Formula: C14H15NO6
SMILES: CC(C)COC(=O)C=CC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 293.27

Physical Properties

Property code	Value	Unit	Source
gf	-184.73	kJ/mol	Joback Method
hf	-495.65	kJ/mol	Joback Method
hfus	39.28	kJ/mol	Joback Method
hvap	84.17	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.256		Crippen Method
mcvol	212.360	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook
tb	859.52	K	Joback Method
tc	1095.01	K	Joback Method
tf	554.33	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.48	J/mol×K	859.52	Joback Method
cpg	626.85	J/mol×K	898.77	Joback Method
cpg	637.14	J/mol×K	938.02	Joback Method
cpg	646.38	J/mol×K	977.26	Joback Method
cpg	654.60	J/mol×K	1016.51	Joback Method
cpg	661.84	J/mol×K	1055.76	Joback Method
cpg	668.14	J/mol×K	1095.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348187&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume