Fumaric acid, butyl 3-nitrophenyl ester

Inchi: InChI=1S/C14H15NO6/c1-2-3-9-20-13(16)7-8-14(17)21-12-6-4-5-11(10-12)15(18)19/h4-8
InchiKey: QFKRHGWEAMGWNC-BQYQJAHWSA-N
Formula: C14H15NO6
SMILES: CCCCOC(=O)C=CC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 293.27

Physical Properties

Property code	Value	Unit	Source
gf	-182.29	kJ/mol	Joback Method
hf	-490.37	kJ/mol	Joback Method
hfus	42.80	kJ/mol	Joback Method
hvap	84.56	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.400		Crippen Method
mcvol	212.360	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	859.96	K	Joback Method
tc	1092.02	K	Joback Method
tf	569.33	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.89	J/mol×K	859.96	Joback Method
cpg	626.13	J/mol×K	898.64	Joback Method
cpg	636.32	J/mol×K	937.31	Joback Method
cpg	645.51	J/mol×K	975.99	Joback Method
cpg	653.73	J/mol×K	1014.66	Joback Method
cpg	661.00	J/mol×K	1053.34	Joback Method
cpg	667.37	J/mol×K	1092.02	Joback Method

Sources

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=U348188&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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