Fumaric acid, 3-nitrophenyl pentyl ester

Inchi: InChI=1S/C15H17NO6/c1-2-3-4-10-21-14(17)8-9-15(18)22-13-7-5-6-12(11-13)16(19)20/
InchiKey: RJOFSOVMAPRYIW-CMDGGOBGSA-N
Formula: C15H17NO6
SMILES: CCCCCOC(=O)C=CC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 307.30

Physical Properties

Property code	Value	Unit	Source
gf	-173.87	kJ/mol	Joback Method
hf	-511.01	kJ/mol	Joback Method
hfus	45.39	kJ/mol	Joback Method
hvap	86.78	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	2.790		Crippen Method
mcvol	226.450	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2445.00		NIST Webbook
tb	882.84	K	Joback Method
tc	1112.43	K	Joback Method
tf	580.60	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.42	J/mol×K	882.84	Joback Method
cpg	681.91	J/mol×K	921.11	Joback Method
cpg	692.35	J/mol×K	959.37	Joback Method
cpg	701.77	J/mol×K	997.64	Joback Method
cpg	710.19	J/mol×K	1035.90	Joback Method
cpg	717.66	J/mol×K	1074.17	Joback Method
cpg	724.22	J/mol×K	1112.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348189&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

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