Fumaric acid, hexyl 3-nitrophenyl ester

Inchi: InChI=1S/C16H19NO6/c1-2-3-4-5-11-22-15(18)9-10-16(19)23-14-8-6-7-13(12-14)17(20)
InchiKey: UIOWUROIBOULOM-MDZDMXLPSA-N
Formula: C16H19NO6
SMILES: CCCCCCOC(=O)C=CC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 321.33

Physical Properties

Property code	Value	Unit	Source
gf	-165.45	kJ/mol	Joback Method
hf	-531.65	kJ/mol	Joback Method
hfus	47.98	kJ/mol	Joback Method
hvap	89.01	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.180		Crippen Method
mcvol	240.540	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	2554.00		NIST Webbook
tb	905.72	K	Joback Method
tc	1133.55	K	Joback Method
tf	591.87	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.77	J/mol×K	905.72	Joback Method
cpg	738.50	J/mol×K	943.69	Joback Method
cpg	749.14	J/mol×K	981.66	Joback Method
cpg	758.74	J/mol×K	1019.64	Joback Method
cpg	767.34	J/mol×K	1057.61	Joback Method
cpg	774.96	J/mol×K	1095.58	Joback Method
cpg	781.66	J/mol×K	1133.55	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=U348191&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume