Fumaric acid, 2-nitrophenyl 2-ethylhexyl ester

Inchi: InChI=1S/C18H23NO6/c1-3-5-8-14(4-2)13-24-17(20)11-12-18(21)25-16-10-7-6-9-15(16)
InchiKey: ZKOHDLBDAJJPOZ-VAWYXSNFSA-N
Formula: C18H23NO6
SMILES: CCCCC(CC)COC(=O)C=CC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 349.38

Physical Properties

Property code	Value	Unit	Source
gf	-151.05	kJ/mol	Joback Method
hf	-578.21	kJ/mol	Joback Method
hfus	49.64	kJ/mol	Joback Method
hvap	93.07	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.816		Crippen Method
mcvol	268.720	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2562.00		NIST Webbook
rinpol	2562.00		NIST Webbook
tb	951.04	K	Joback Method
tc	1179.63	K	Joback Method
tf	599.41	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.21	J/mol×K	951.04	Joback Method
cpg	854.37	J/mol×K	989.14	Joback Method
cpg	865.37	J/mol×K	1027.24	Joback Method
cpg	875.24	J/mol×K	1065.34	Joback Method
cpg	884.05	J/mol×K	1103.43	Joback Method
cpg	891.82	J/mol×K	1141.53	Joback Method
cpg	898.62	J/mol×K	1179.63	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=U405796&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