Fumaric acid, di(4-nitrophenyl) ester

Inchi: InChI=1S/C16H10N2O8/c19-15(25-13-5-1-11(2-6-13)17(21)22)9-10-16(20)26-14-7-3-12(
InchiKey: ZLNCGIAXVWNFRX-MDZDMXLPSA-N
Formula: C16H10N2O8
SMILES: O=C(C=CC(=O)Oc1ccc([N+](=O)[O-])cc1)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 358.26

Physical Properties

Property code	Value	Unit	Source
gf	-27.12	kJ/mol	Joback Method
hf	-317.35	kJ/mol	Joback Method
hfus	53.00	kJ/mol	Joback Method
hvap	108.54	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	2.570		Crippen Method
mcvol	234.200	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	3135.00		NIST Webbook
rinpol	3135.00		NIST Webbook
tb	1089.22	K	Joback Method
tc	1364.83	K	Joback Method
tf	774.42	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.96	J/mol×K	1089.22	Joback Method
cpg	698.47	J/mol×K	1135.15	Joback Method
cpg	702.80	J/mol×K	1181.09	Joback Method
cpg	706.03	J/mol×K	1227.02	Joback Method
cpg	708.23	J/mol×K	1272.96	Joback Method
cpg	709.50	J/mol×K	1318.89	Joback Method
cpg	709.91	J/mol×K	1364.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405792&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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