Fumaric acid, isohexyl 3-nitrophenyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-167.89	kJ/mol	Joback Method
hf	-536.93	kJ/mol	Joback Method
hfus	44.46	kJ/mol	Joback Method
hvap	88.62	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.036		Crippen Method
mcvol	240.540	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
tb	905.28	K	Joback Method
tc	1135.85	K	Joback Method
tf	576.87	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.31	J/mol×K	905.28	Joback Method
cpg	739.14	J/mol×K	943.71	Joback Method
cpg	749.84	J/mol×K	982.14	Joback Method
cpg	759.46	J/mol×K	1020.56	Joback Method
cpg	768.03	J/mol×K	1058.99	Joback Method
cpg	775.61	J/mol×K	1097.42	Joback Method
cpg	782.22	J/mol×K	1135.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348190&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