Fumaric acid, 3-nitrophenyl propyl ester

Inchi: InChI=1S/C13H13NO6/c1-2-8-19-12(15)6-7-13(16)20-11-5-3-4-10(9-11)14(17)18/h3-7,9H
InchiKey: ZSBBMWWYSOASOZ-VOTSOKGWSA-N
Formula: C13H13NO6
SMILES: CCCOC(=O)C=CC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 279.25

Physical Properties

Property code	Value	Unit	Source
gf	-190.71	kJ/mol	Joback Method
hf	-469.73	kJ/mol	Joback Method
hfus	40.21	kJ/mol	Joback Method
hvap	82.33	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.010		Crippen Method
mcvol	198.270	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook
tb	837.08	K	Joback Method
tc	1072.26	K	Joback Method
tf	558.06	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.27	J/mol×K	837.08	Joback Method
cpg	571.19	J/mol×K	876.28	Joback Method
cpg	581.09	J/mol×K	915.47	Joback Method
cpg	590.01	J/mol×K	954.67	Joback Method
cpg	597.97	J/mol×K	993.87	Joback Method
cpg	605.01	J/mol×K	1033.06	Joback Method
cpg	611.15	J/mol×K	1072.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348186&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