Fumaric acid, 2-nitrophenyl dec-2-yl ester

Inchi: InChI=1S/C20H27NO6/c1-3-4-5-6-7-8-11-16(2)26-19(22)14-15-20(23)27-18-13-10-9-12-
InchiKey: DENDZTVAWQNIMC-CCEZHUSRSA-N
Formula: C20H27NO6
SMILES: CCCCCCCCC(C)OC(=O)C=CC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 377.43

Physical Properties

Property code	Value	Unit	Source
gf	-134.21	kJ/mol	Joback Method
hf	-619.49	kJ/mol	Joback Method
hfus	54.82	kJ/mol	Joback Method
hvap	97.52	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	4.739		Crippen Method
mcvol	296.900	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	996.80	K	Joback Method
tc	1226.73	K	Joback Method
tf	621.95	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.72	J/mol×K	996.80	Joback Method
cpg	972.18	J/mol×K	1035.12	Joback Method
cpg	983.41	J/mol×K	1073.44	Joback Method
cpg	993.47	J/mol×K	1111.76	Joback Method
cpg	1002.42	J/mol×K	1150.09	Joback Method
cpg	1010.31	J/mol×K	1188.41	Joback Method
cpg	1017.20	J/mol×K	1226.73	Joback Method

Sources

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=U405800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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