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

Inchi: InChI=1S/C17H21NO6/c1-3-4-5-8-13(2)23-16(19)11-12-17(20)24-15-10-7-6-9-14(15)18(
InchiKey: PNESYOKPZPCUDC-VAWYXSNFSA-N
Formula: C17H21NO6
SMILES: CCCCCC(C)OC(=O)C=CC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 335.35

Physical Properties

Property code	Value	Unit	Source
gf	-159.47	kJ/mol	Joback Method
hf	-557.57	kJ/mol	Joback Method
hfus	47.05	kJ/mol	Joback Method
hvap	90.85	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.568		Crippen Method
mcvol	254.630	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	928.16	K	Joback Method
tc	1157.35	K	Joback Method
tf	588.14	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.41	J/mol×K	928.16	Joback Method
cpg	796.41	J/mol×K	966.36	Joback Method
cpg	807.27	J/mol×K	1004.56	Joback Method
cpg	817.03	J/mol×K	1042.75	Joback Method
cpg	825.73	J/mol×K	1080.95	Joback Method
cpg	833.42	J/mol×K	1119.15	Joback Method
cpg	840.14	J/mol×K	1157.35	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=U405794&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