Fumaric acid, 4-nitrophenyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C21H15NO6/c23-20(27-14-15-5-6-16-3-1-2-4-17(16)13-15)11-12-21(24)28-19-
InchiKey: NZFWELYRBDKACP-VAWYXSNFSA-N
Formula: C21H15NO6
SMILES: O=C(C=CC(=O)Oc1ccc([N+](=O)[O-])cc1)OCc1ccc2ccccc2c1
Mol. weight [g/mol]: 377.35

Physical Properties

Property code	Value	Unit	Source
gf	86.08	kJ/mol	Joback Method
hf	-218.72	kJ/mol	Joback Method
hfus	51.61	kJ/mol	Joback Method
hvap	104.72	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	3.953		Crippen Method
mcvol	267.770	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	3264.00		NIST Webbook
rinpol	3264.00		NIST Webbook
tb	1070.76	K	Joback Method
tc	1335.57	K	Joback Method
tf	719.86	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.75	J/mol×K	1070.76	Joback Method
cpg	826.21	J/mol×K	1114.89	Joback Method
cpg	834.82	J/mol×K	1159.03	Joback Method
cpg	842.73	J/mol×K	1203.16	Joback Method
cpg	850.08	J/mol×K	1247.30	Joback Method
cpg	856.99	J/mol×K	1291.43	Joback Method
cpg	863.59	J/mol×K	1335.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405791&Units=SI

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