Fumaric acid, naphth-1-yl hex-4-yn-3-yl ester

Inchi: InChI=1S/C20H18O4/c1-3-8-16(4-2)23-19(21)13-14-20(22)24-18-12-7-10-15-9-5-6-11-17
InchiKey: JETJNBUPCORCLC-BUHFOSPRSA-N
Formula: C20H18O4
SMILES: CC#CC(CC)OC(=O)C=CC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 322.35

Physical Properties

Property code	Value	Unit	Source
gf	139.69	kJ/mol	Joback Method
hf	-145.36	kJ/mol	Joback Method
hfus	43.60	kJ/mol	Joback Method
hvap	84.73	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	3.647		Crippen Method
mcvol	251.420	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	872.94	K	Joback Method
tc	1112.51	K	Joback Method
tf	617.14	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.85	J/mol×K	872.94	Joback Method
cpg	736.49	J/mol×K	912.87	Joback Method
cpg	749.07	J/mol×K	952.80	Joback Method
cpg	760.66	J/mol×K	992.73	Joback Method
cpg	771.34	J/mol×K	1032.65	Joback Method
cpg	781.19	J/mol×K	1072.58	Joback Method
cpg	790.30	J/mol×K	1112.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405809&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