Fumaric acid, naphth-1-yl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C20H12ClFO4/c21-15-8-4-9-16(22)20(15)26-19(24)12-11-18(23)25-17-10-3-6-

InchiKey: UKLIXFSFAODRDU-VAWYXSNFSA-N

Formula: C20H12ClFO4

SMILES: O=C(C=CC(=O)Oc1cccc2ccccc12)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 370.76

Physical Properties

Property code	Value	Unit	Source
gf	-174.26	kJ/mol	Joback Method
hf	-410.64	kJ/mol	Joback Method
hfus	44.54	kJ/mol	Joback Method
hvap	90.13	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	4.699		Crippen Method
mcvol	250.270	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	2859.00		NIST Webbook
rinpol	2859.00		NIST Webbook
tb	937.72	K	Joback Method
tc	1184.08	K	Joback Method
tf	608.01	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.65	J/mol×K	937.72	Joback Method
cpg	709.01	J/mol×K	978.78	Joback Method
cpg	718.43	J/mol×K	1019.84	Joback Method
cpg	726.98	J/mol×K	1060.90	Joback Method
cpg	734.76	J/mol×K	1101.96	Joback Method
cpg	741.87	J/mol×K	1143.02	Joback Method
cpg	748.39	J/mol×K	1184.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405813&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