Fumaric acid, naphth-2-yl 2-fluorophenyl ester

Inchi: InChI=1S/C20H13FO4/c21-17-7-3-4-8-18(17)25-20(23)12-11-19(22)24-16-10-9-14-5-1-2
InchiKey: GHQVPKBAQRPWRO-VAWYXSNFSA-N
Formula: C20H13FO4
SMILES: O=C(C=CC(=O)Oc1ccccc1F)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 336.31

Physical Properties

Property code	Value	Unit	Source
gf	-152.70	kJ/mol	Joback Method
hf	-383.43	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	85.08	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.046		Crippen Method
mcvol	238.030	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	2767.00		NIST Webbook
rinpol	2767.00		NIST Webbook
tb	895.31	K	Joback Method
tc	1138.45	K	Joback Method
tf	565.57	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.87	J/mol×K	895.31	Joback Method
cpg	692.46	J/mol×K	935.83	Joback Method
cpg	703.03	J/mol×K	976.36	Joback Method
cpg	712.67	J/mol×K	1016.88	Joback Method
cpg	721.47	J/mol×K	1057.41	Joback Method
cpg	729.52	J/mol×K	1097.93	Joback Method
cpg	736.93	J/mol×K	1138.45	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=U405830&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