

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

Inchi: InChI=1S/C20H13FO4/c21-16-9-3-4-10-18(16)25-20(23)13-12-19(22)24-17-11-5-7-14-6-
InchiKey: CTVFZJUGOLYCFR-OUKQBFOZSA-N
Formula: C20H13FO4
SMILES: O=C(C=CC(=O)Oc1cccc2ccccc12)Oc1cccc1F
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
mvol	238.030	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook
tb	895.31	K	Joback Method
tc	1138.45	K	Joback Method
tf	565.57	K	Joback Method
vc	0.907	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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