Fumaric acid, monoamide, N-benzyl-N-phenethyl-, 3-fluorophenyl ester

Inchi: InChI=1S/C25H22FNO3/c26-22-12-7-13-23(18-22)30-25(29)15-14-24(28)27(19-21-10-5-
InchiKey: NELJQPRPADOPOH-CCEZHUSRSA-N
Formula: C25H22FNO3
SMILES: O=C(C=CC(=O)N(CCc1ccccc1)Cc1ccccc1)Oc1cccc(F)c1
Mol. weight [g/mol]: 403.45

Physical Properties

Property code	Value	Unit	Source
gf	120.57	kJ/mol	Joback Method
hf	-229.95	kJ/mol	Joback Method
hfus	52.93	kJ/mol	Joback Method
hvap	95.82	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.559		Crippen Method
mcvol	308.290	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	3342.00		NIST Webbook
rinpol	3342.00		NIST Webbook
tb	1002.45	K	Joback Method
tc	1244.79	K	Joback Method
tf	613.36	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.35	J/mol×K	1002.45	Joback Method
cpg	975.09	J/mol×K	1042.84	Joback Method
cpg	986.80	J/mol×K	1083.23	Joback Method
cpg	997.62	J/mol×K	1123.62	Joback Method
cpg	1007.70	J/mol×K	1164.01	Joback Method
cpg	1017.17	J/mol×K	1204.40	Joback Method
cpg	1026.17	J/mol×K	1244.79	Joback Method

Sources

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=U357492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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