Fumaric acid, monoamide, N-(2-fluorophenyl)-, neopentyl ester

Inchi: InChI=1S/C15H18FNO3/c1-15(2,3)10-20-14(19)9-8-13(18)17-12-7-5-4-6-11(12)16/h4-9H

InchiKey: LXIIHKZXZJKXMY-CMDGGOBGSA-N

Formula: C15H18FNO3

SMILES: CC(C)(C)COC(=O)C=CC(=O)Nc1ccccc1F

Mol. weight [g/mol]: 279.31

Physical Properties

Property code	Value	Unit	Source
gf	-207.00	kJ/mol	Joback Method
hf	-519.42	kJ/mol	Joback Method
hfus	33.61	kJ/mol	Joback Method
hvap	72.11	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.910		Crippen Method
mcvol	214.910	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	2149.00		NIST Webbook
tb	754.79	K	Joback Method
tc	968.71	K	Joback Method
tf	470.43	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.69	J/mol×K	754.79	Joback Method
cpg	620.34	J/mol×K	790.44	Joback Method
cpg	633.02	J/mol×K	826.10	Joback Method
cpg	644.80	J/mol×K	861.75	Joback Method
cpg	655.72	J/mol×K	897.40	Joback Method
cpg	665.87	J/mol×K	933.06	Joback Method
cpg	675.29	J/mol×K	968.71	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=U357513&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