Fumaric acid, monoamide, N-methyl-N-phenyl-, 2-biphenyl ester

Inchi: InChI=1S/C23H19NO3/c1-24(19-12-6-3-7-13-19)22(25)16-17-23(26)27-21-15-9-8-14-20(

InchiKey: XXVOJHZYCPTKNX-WUKNDPDISA-N

Formula: C23H19NO3

SMILES: CN(C(=O)C=CC(=O)Oc1ccccc1-c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 357.40

Physical Properties

Property code	Value	Unit	Source
gf	298.54	kJ/mol	Joback Method
hf	7.44	kJ/mol	Joback Method
hfus	44.67	kJ/mol	Joback Method
hvap	92.19	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.478		Crippen Method
mcvol	278.340	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	3063.00		NIST Webbook
rinpol	3063.00		NIST Webbook
tb	957.42	K	Joback Method
tc	1210.52	K	Joback Method
tf	590.23	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.27	J/mol×K	957.42	Joback Method
cpg	851.17	J/mol×K	999.60	Joback Method
cpg	862.93	J/mol×K	1041.79	Joback Method
cpg	873.67	J/mol×K	1083.97	Joback Method
cpg	883.56	J/mol×K	1126.15	Joback Method
cpg	892.73	J/mol×K	1168.34	Joback Method
cpg	901.33	J/mol×K	1210.52	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357462&Units=SI

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