Fumaric acid, monoamide, N,N-dimethyl-, 2-biphenyl ester

Inchi: InChI=1S/C18H17NO3/c1-19(2)17(20)12-13-18(21)22-16-11-7-6-10-15(16)14-8-4-3-5-9-
InchiKey: HNISNVWQVVQBKY-OUKQBFOZSA-N
Formula: C18H17NO3
SMILES: CN(C)C(=O)C=CC(=O)Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]: 295.33

Physical Properties

Property code	Value	Unit	Source
gf	144.03	kJ/mol	Joback Method
hf	-125.89	kJ/mol	Joback Method
hfus	37.68	kJ/mol	Joback Method
hvap	78.78	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	2.903		Crippen Method
mcvol	231.650	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	2594.00		NIST Webbook
tb	816.34	K	Joback Method
tc	1052.04	K	Joback Method
tf	507.46	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.74	J/mol×K	816.34	Joback Method
cpg	669.76	J/mol×K	855.62	Joback Method
cpg	682.60	J/mol×K	894.91	Joback Method
cpg	694.36	J/mol×K	934.19	Joback Method
cpg	705.11	J/mol×K	973.47	Joback Method
cpg	714.96	J/mol×K	1012.75	Joback Method
cpg	723.99	J/mol×K	1052.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357461&Units=SI
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

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