

Fumaric acid, monoamide, N-methyl-N-phenyl-, 3-methylphenyl ester

Inchi:	InChI=1S/C18H17NO3/c1-14-7-6-10-16(13-14)22-18(21)12-11-17(20)19(2)15-8-4-3-5-9-
InchiKey:	NHVALAHENMCJLC-VAWYXSNFSA-N
Formula:	C18H17NO3
SMILES:	<chem>Cc1cccc(OC(=O)C=CC(=O)N(C)c2ccccc2)c1</chem>
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	-3.87		Crippen Method
logp	3.120		Crippen Method
mcvol	231.650	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpola	2587.00		NIST Webbook
rinpola	2587.00		NIST Webbook
tb	816.34	K	Joback Method
tc	1052.04	K	Joback Method
tf	507.46	K	Joback Method
vc	0.856	m ³ /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=U357455&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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