Fumaric acid, monoamide, N-methallyl-, 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C16H19NO5/c1-11(2)10-17-14(18)8-9-15(19)22-16-12(20-3)6-5-7-13(16)21-4/h

InchiKey: UEZMHPIFWJTKEG-CMDGGOBGSA-N

Formula: C16H19NO5

SMILES: C=C(C)CNC(=O)C=CC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 305.33

Physical Properties

Property code	Value	Unit	Source
gf	-146.95	kJ/mol	Joback Method
hf	-495.47	kJ/mol	Joback Method
hfus	39.93	kJ/mol	Joback Method
hvap	81.34	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	1.858		Crippen Method
mcvol	234.670	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	2623.00		NIST Webbook
tb	828.01	K	Joback Method
tc	1042.08	K	Joback Method
tf	519.95	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.85	J/mol×K	828.01	Joback Method
cpg	690.86	J/mol×K	863.69	Joback Method
cpg	702.85	J/mol×K	899.37	Joback Method
cpg	713.82	J/mol×K	935.04	Joback Method
cpg	723.79	J/mol×K	970.72	Joback Method
cpg	732.78	J/mol×K	1006.40	Joback Method
cpg	740.80	J/mol×K	1042.08	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=U357459&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