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

Inchi: InChI=1S/C15H17NO5/c1-4-10-16-13(17)8-9-14(18)21-15-11(19-2)6-5-7-12(15)20-3/h4-9

InchiKey: PGCWKNKGGMFTEF-CMDGGOBGSA-N

Formula: C15H17NO5

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

Mol. weight [g/mol]: 291.30

Physical Properties

Property code	Value	Unit	Source
gf	-146.82	kJ/mol	Joback Method
hf	-465.04	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	79.03	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	1.468		Crippen Method
mcvol	220.580	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	2543.00		NIST Webbook
tb	805.25	K	Joback Method
tc	1018.58	K	Joback Method
tf	522.64	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.79	J/mol×K	805.25	Joback Method
cpg	635.37	J/mol×K	840.80	Joback Method
cpg	646.98	J/mol×K	876.36	Joback Method
cpg	657.62	J/mol×K	911.91	Joback Method
cpg	667.32	J/mol×K	947.47	Joback Method
cpg	676.07	J/mol×K	983.02	Joback Method
cpg	683.89	J/mol×K	1018.58	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=U357458&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

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