Fumaric acid, monoamide, N-(2-ethylphenyl)-, isopropyl ester

Inchi: InChI=1S/C15H19NO3/c1-4-12-7-5-6-8-13(12)16-14(17)9-10-15(18)19-11(2)3/h5-11H,4H

InchiKey: VLCIZJOPVOGLQB-MDZDMXLPSA-N

Formula: C15H19NO3

SMILES: CCc1ccccc1NC(=O)C=CC(=O)OC(C)C

Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
gf	-17.47	kJ/mol	Joback Method
hf	-319.84	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.695		Crippen Method
mcvol	213.140	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	2192.00		NIST Webbook
rinpol	2192.00		NIST Webbook
tb	758.31	K	Joback Method
tc	973.91	K	Joback Method
tf	452.42	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.28	J/mol×K	758.31	Joback Method
cpg	611.46	J/mol×K	794.24	Joback Method
cpg	624.66	J/mol×K	830.18	Joback Method
cpg	636.91	J/mol×K	866.11	Joback Method
cpg	648.27	J/mol×K	902.04	Joback Method
cpg	658.77	J/mol×K	937.98	Joback Method
cpg	668.46	J/mol×K	973.91	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=U357523&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