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

Inchi: InChI=1S/C17H23NO3/c1-4-8-13(3)21-17(20)12-11-16(19)18-15-10-7-6-9-14(15)5-2/h6-1

InchiKey: AIXXNEVYBPOHAY-VAWYXSNFSA-N

Formula: C17H23NO3

SMILES: CCCC(C)OC(=O)C=CC(=O)Nc1ccccc1CC

Mol. weight [g/mol]: 289.37

Physical Properties

Property code	Value	Unit	Source
gf	-0.63	kJ/mol	Joback Method
hf	-361.12	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.476		Crippen Method
mcvol	241.320	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
tb	804.07	K	Joback Method
tc	1015.28	K	Joback Method
tf	474.96	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.15	J/mol×K	804.07	Joback Method
cpg	722.92	J/mol×K	839.27	Joback Method
cpg	736.68	J/mol×K	874.47	Joback Method
cpg	749.47	J/mol×K	909.68	Joback Method
cpg	761.34	J/mol×K	944.88	Joback Method
cpg	772.34	J/mol×K	980.08	Joback Method
cpg	782.51	J/mol×K	1015.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357495&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

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