Fumaric acid, monoamide, N-(4-chlorophenyl)-, 2-pentyl ester

Inchi: InChI=1S/C15H18ClNO3/c1-3-4-11(2)20-15(19)10-9-14(18)17-13-7-5-12(16)6-8-13/h5-1

InchiKey: NAMGGIHOZXIRHQ-MDZDMXLPSA-N

Formula: C15H18ClNO3

SMILES: CCCC(C)OC(=O)C=CC(=O)Nc1ccc(Cl)cc1

Mol. weight [g/mol]: 295.76

Physical Properties

Property code	Value	Unit	Source
gf	-29.40	kJ/mol	Joback Method
hf	-335.58	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.566		Crippen Method
mcvol	225.380	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	2577.00		NIST Webbook
rinpol	2577.00		NIST Webbook
tb	795.74	K	Joback Method
tc	1014.50	K	Joback Method
tf	482.34	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.93	J/mol×K	795.74	Joback Method
cpg	634.96	J/mol×K	832.20	Joback Method
cpg	647.03	J/mol×K	868.66	Joback Method
cpg	658.19	J/mol×K	905.12	Joback Method
cpg	668.48	J/mol×K	941.58	Joback Method
cpg	677.95	J/mol×K	978.04	Joback Method
cpg	686.65	J/mol×K	1014.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357497&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