Fumaric acid, monoamide, N-methyl-N-phenyl-, 2-pentyl ester

Inchi: InChI=1S/C16H21NO3/c1-4-8-13(2)20-16(19)12-11-15(18)17(3)14-9-6-5-7-10-14/h5-7,9-

InchiKey: KDOUYXLSDOUHBY-VAWYXSNFSA-N

Formula: C16H21NO3

SMILES: CCCC(C)OC(=O)C=CC(=O)N(C)c1ccccc1

Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
gf	21.97	kJ/mol	Joback Method
hf	-314.95	kJ/mol	Joback Method
hfus	35.32	kJ/mol	Joback Method
hvap	71.00	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.937		Crippen Method
mcvol	227.230	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	738.48	K	Joback Method
tc	948.35	K	Joback Method
tf	430.98	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.18	J/mol×K	738.48	Joback Method
cpg	653.62	J/mol×K	773.46	Joback Method
cpg	668.02	J/mol×K	808.44	Joback Method
cpg	681.43	J/mol×K	843.41	Joback Method
cpg	693.90	J/mol×K	878.39	Joback Method
cpg	705.50	J/mol×K	913.37	Joback Method
cpg	716.27	J/mol×K	948.35	Joback Method

Sources

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=U357493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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