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

Inchi: InChI=1S/C19H27NO3/c1-4-6-10-16(5-2)15-23-19(22)14-13-18(21)20(3)17-11-8-7-9-12-
InchiKey: XSYLUJMUMHTSKN-BUHFOSPRSA-N
Formula: C19H27NO3
SMILES: CCCCC(CC)COC(=O)C=CC(=O)N(C)c1ccccc1
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
gf	47.23	kJ/mol	Joback Method
hf	-376.87	kJ/mol	Joback Method
hfus	43.09	kJ/mol	Joback Method
hvap	77.68	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.965		Crippen Method
mcvol	269.500	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2497.00		NIST Webbook
rinpol	2497.00		NIST Webbook
tb	807.12	K	Joback Method
tc	1011.91	K	Joback Method
tf	464.79	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.26	J/mol×K	807.12	Joback Method
cpg	823.42	J/mol×K	841.25	Joback Method
cpg	838.51	J/mol×K	875.38	Joback Method
cpg	852.60	J/mol×K	909.51	Joback Method
cpg	865.75	J/mol×K	943.64	Joback Method
cpg	878.02	J/mol×K	977.77	Joback Method
cpg	889.46	J/mol×K	1011.91	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=U357505&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