Fumaric acid, monoamide, N-benzyl-N-phenethyl-, 2-ethylhexyl ester

Inchi: InChI=1S/C27H35NO3/c1-3-5-12-23(4-2)22-31-27(30)18-17-26(29)28(21-25-15-10-7-11-

InchiKey: IQIQNWWAYNDDFW-ISLYRVAYSA-N

Formula: C27H35NO3

SMILES: CCCCC(CC)COC(=O)C=CC(=O)N(CCc1ccccc1)Cc1ccccc1

Mol. weight [g/mol]: 421.57

Physical Properties

Property code	Value	Unit	Source
gf	227.00	kJ/mol	Joback Method
hf	-305.46	kJ/mol	Joback Method
hfus	57.85	kJ/mol	Joback Method
hvap	97.76	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.574		Crippen Method
mcvol	358.460	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	3384.00		NIST Webbook
tb	1016.84	K	Joback Method
tc	1247.41	K	Joback Method
tf	581.37	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.08	J/mol×K	1016.84	Joback Method
cpg	1202.90	J/mol×K	1055.27	Joback Method
cpg	1217.61	J/mol×K	1093.70	Joback Method
cpg	1231.32	J/mol×K	1132.13	Joback Method
cpg	1244.16	J/mol×K	1170.56	Joback Method
cpg	1256.27	J/mol×K	1208.99	Joback Method
cpg	1267.76	J/mol×K	1247.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357510&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