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

Inchi: InChI=1S/C24H29NO3/c1-3-10-20(2)28-24(27)16-15-23(26)25(19-22-13-8-5-9-14-22)18-

InchiKey: XFKHNKCVSDNYAB-FOCLMDBBSA-N

Formula: C24H29NO3

SMILES: CCCC(C)OC(=O)C=CC(=O)N(CCc1ccccc1)Cc1ccccc1

Mol. weight [g/mol]: 379.49

Physical Properties

Property code	Value	Unit	Source
gf	201.74	kJ/mol	Joback Method
hf	-243.54	kJ/mol	Joback Method
hfus	50.08	kJ/mol	Joback Method
hvap	91.08	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.546		Crippen Method
mcvol	316.190	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	3047.00		NIST Webbook
tb	948.20	K	Joback Method
tc	1174.48	K	Joback Method
tf	547.56	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.41	J/mol×K	948.20	Joback Method
cpg	1019.61	J/mol×K	985.91	Joback Method
cpg	1033.66	J/mol×K	1023.63	Joback Method
cpg	1046.70	J/mol×K	1061.34	Joback Method
cpg	1058.81	J/mol×K	1099.05	Joback Method
cpg	1070.11	J/mol×K	1136.76	Joback Method
cpg	1080.71	J/mol×K	1174.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357500&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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