Fumaric acid, monoamide, N-benzyl-N-phenethyl-, isopropyl ester

Inchi: InChI=1S/C22H25NO3/c1-18(2)26-22(25)14-13-21(24)23(17-20-11-7-4-8-12-20)16-15-19
InchiKey: XXPGSJYLWLFSBH-BUHFOSPRSA-N
Formula: C22H25NO3
SMILES: CC(C)OC(=O)C=CC(=O)N(CCc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]: 351.44

Physical Properties

Property code	Value	Unit	Source
gf	184.90	kJ/mol	Joback Method
hf	-202.26	kJ/mol	Joback Method
hfus	44.90	kJ/mol	Joback Method
hvap	86.63	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.766		Crippen Method
mcvol	288.010	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2831.00		NIST Webbook
rinpol	2831.00		NIST Webbook
tb	902.44	K	Joback Method
tc	1130.09	K	Joback Method
tf	525.02	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.77	J/mol×K	902.44	Joback Method
cpg	900.68	J/mol×K	940.38	Joback Method
cpg	914.43	J/mol×K	978.32	Joback Method
cpg	927.12	J/mol×K	1016.27	Joback Method
cpg	938.86	J/mol×K	1054.21	Joback Method
cpg	949.74	J/mol×K	1092.15	Joback Method
cpg	959.87	J/mol×K	1130.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357528&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

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