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

Inchi: InChI=1S/C26H20F5NO3/c27-22-19(23(28)25(30)26(31)24(22)29)16-35-21(34)12-11-20
InchiKey: ZACTUGKRNDVQCT-VAWYXSNFSA-N
Formula: C26H20F5NO3
SMILES: O=C(C=CC(=O)N(CCc1ccccc1)Cc1ccccc1)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 489.43

Physical Properties

Property code	Value	Unit	Source
gf	-688.77	kJ/mol	Joback Method
hf	-1080.91	kJ/mol	Joback Method
hfus	66.28	kJ/mol	Joback Method
hvap	97.43	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	5.253		Crippen Method
mcvol	329.460	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	3268.00		NIST Webbook
rinpol	3268.00		NIST Webbook
tb	1042.33	K	Joback Method
tc	1276.70	K	Joback Method
tf	677.07	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1042.75	J/mol×K	1042.33	Joback Method
cpg	1054.02	J/mol×K	1081.39	Joback Method
cpg	1064.26	J/mol×K	1120.45	Joback Method
cpg	1073.58	J/mol×K	1159.51	Joback Method
cpg	1082.07	J/mol×K	1198.58	Joback Method
cpg	1089.84	J/mol×K	1237.64	Joback Method
cpg	1096.99	J/mol×K	1276.70	Joback Method

Sources

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=U357453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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