Fumaric acid, monoamide, N-benzyl-N-phenethyl-, 3,5-difluorophenyl ester

Othernames: Fumaric acid, monoamide, N-benzyl-N-phenethyl-, 3,5-fluorophenyl ester
Inchi: InChI=1S/C25H21F2NO3/c26-21-15-22(27)17-23(16-21)31-25(30)12-11-24(29)28(18-20
InchiKey: XBIHRQSOOJOZQY-VAWYXSNFSA-N
Formula: C25H21F2NO3
SMILES: O=C(C=CC(=O)N(CCc1ccccc1)Cc1ccccc1)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 421.44

Physical Properties

Property code	Value	Unit	Source
gf	-83.87	kJ/mol	Joback Method
hf	-437.53	kJ/mol	Joback Method
hfus	55.62	kJ/mol	Joback Method
hvap	95.67	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	4.698		Crippen Method
mcvol	310.060	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	3246.00		NIST Webbook
rinpol	3246.00		NIST Webbook
tb	1006.70	K	Joback Method
tc	1244.83	K	Joback Method
tf	626.47	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.75	J/mol×K	1006.70	Joback Method
cpg	979.97	J/mol×K	1046.39	Joback Method
cpg	991.18	J/mol×K	1086.08	Joback Method
cpg	1001.51	J/mol×K	1125.76	Joback Method
cpg	1011.07	J/mol×K	1165.45	Joback Method
cpg	1020.00	J/mol×K	1205.14	Joback Method
cpg	1028.43	J/mol×K	1244.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357411&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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