2,4,5-Trifluoro-3-methoxybenzamide, N-(1-naphthyl)-

Inchi: InChI=1S/C18H12F3NO2/c1-24-17-15(20)12(9-13(19)16(17)21)18(23)22-14-8-4-6-10-5-2
InchiKey: DSTHAANBQHQFGV-UHFFFAOYSA-N
Formula: C18H12F3NO2
SMILES: COc1c(F)c(F)cc(C(=O)Nc2cccc3ccccc23)c1F
Mol. weight [g/mol]: 331.29

Physical Properties

Property code	Value	Unit	Source
gf	-344.96	kJ/mol	Joback Method
hf	-587.73	kJ/mol	Joback Method
hfus	42.66	kJ/mol	Joback Method
hvap	78.31	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	4.518		Crippen Method
mcvol	220.230	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
tb	832.75	K	Joback Method
tc	1057.28	K	Joback Method
tf	567.35	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.09	J/mol×K	832.75	Joback Method
cpg	636.80	J/mol×K	870.17	Joback Method
cpg	647.58	J/mol×K	907.59	Joback Method
cpg	657.48	J/mol×K	945.02	Joback Method
cpg	666.56	J/mol×K	982.44	Joback Method
cpg	674.87	J/mol×K	1019.86	Joback Method
cpg	682.46	J/mol×K	1057.28	Joback Method

Sources

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=U358072&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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