2,6-Difluoro-3-methylbenzamide, N-(1-naphthyl)-

Inchi: InChI=1S/C18H13F2NO/c1-11-9-10-14(19)16(17(11)20)18(22)21-15-8-4-6-12-5-2-3-7-13
InchiKey: WVTRERGGNITXDJ-UHFFFAOYSA-N
Formula: C18H13F2NO
SMILES: Cc1ccc(F)c(C(=O)Nc2cccc3ccccc23)c1F
Mol. weight [g/mol]: 297.30

Physical Properties

Property code	Value	Unit	Source
gf	-35.52	kJ/mol	Joback Method
hf	-247.93	kJ/mol	Joback Method
hfus	38.78	kJ/mol	Joback Method
hvap	76.05	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	4.679		Crippen Method
mcvol	212.590	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	2654.00		NIST Webbook
rinpol	2654.00		NIST Webbook
tb	806.08	K	Joback Method
tc	1040.29	K	Joback Method
tf	532.01	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.43	J/mol×K	806.08	Joback Method
cpg	606.18	J/mol×K	845.11	Joback Method
cpg	617.96	J/mol×K	884.15	Joback Method
cpg	628.84	J/mol×K	923.18	Joback Method
cpg	638.93	J/mol×K	962.22	Joback Method
cpg	648.31	J/mol×K	1001.25	Joback Method
cpg	657.07	J/mol×K	1040.29	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=U358108&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