3,4-Difluorobenzamide, N-pentyl-

Inchi: InChI=1S/C12H15F2NO/c1-2-3-4-7-15-12(16)9-5-6-10(13)11(14)8-9/h5-6,8H,2-4,7H2,1H
InchiKey: XSZZEZIGFDGCHR-UHFFFAOYSA-N
Formula: C12H15F2NO
SMILES: CCCCCNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 227.25

Physical Properties

Property code	Value	Unit	Source
gf	-285.84	kJ/mol	Joback Method
hf	-528.75	kJ/mol	Joback Method
hfus	32.96	kJ/mol	Joback Method
hvap	57.45	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	2.885		Crippen Method
mcvol	171.270	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
tb	613.18	K	Joback Method
tc	805.44	K	Joback Method
tf	380.23	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.32	J/mol×K	613.18	Joback Method
cpg	448.75	J/mol×K	645.22	Joback Method
cpg	461.45	J/mol×K	677.27	Joback Method
cpg	473.45	J/mol×K	709.31	Joback Method
cpg	484.75	J/mol×K	741.35	Joback Method
cpg	495.40	J/mol×K	773.40	Joback Method
cpg	505.41	J/mol×K	805.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358122&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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