Benzamide, 2,5-difluoro-N-(2,5-difluorobenzoyl)-N-undecyl-

Inchi: InChI=1S/C25H29F4NO2/c1-2-3-4-5-6-7-8-9-10-15-30(24(31)20-16-18(26)11-13-22(20)2

InchiKey: ZZVBXYIMHCNDSX-UHFFFAOYSA-N

Formula: C25H29F4NO2

SMILES: CCCCCCCCCCCN(C(=O)c1cc(F)ccc1F)C(=O)c1cc(F)ccc1F

Mol. weight [g/mol]: 451.50

Physical Properties

Property code	Value	Unit	Source
gf	-580.38	kJ/mol	Joback Method
hf	-1074.22	kJ/mol	Joback Method
hfus	65.57	kJ/mol	Joback Method
hvap	90.71	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	7.056		Crippen Method
mcvol	335.790	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	2741.00		NIST Webbook
rinpol	2741.00		NIST Webbook
tb	961.94	K	Joback Method
tc	1177.76	K	Joback Method
tf	609.12	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.61	J/mol×K	961.94	Joback Method
cpg	1103.41	J/mol×K	997.91	Joback Method
cpg	1117.10	J/mol×K	1033.88	Joback Method
cpg	1129.74	J/mol×K	1069.85	Joback Method
cpg	1141.40	J/mol×K	1105.82	Joback Method
cpg	1152.18	J/mol×K	1141.79	Joback Method
cpg	1162.15	J/mol×K	1177.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407612&Units=SI

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