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

Inchi: InChI=1S/C26H31F4NO2/c1-2-3-4-5-6-7-8-9-10-11-16-31(25(32)21-17-19(27)12-14-23(2

InchiKey: WKYDUJRZSDTKOJ-UHFFFAOYSA-N

Formula: C26H31F4NO2

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

Mol. weight [g/mol]: 465.52

Physical Properties

Property code	Value	Unit	Source
gf	-571.96	kJ/mol	Joback Method
hf	-1094.86	kJ/mol	Joback Method
hfus	68.16	kJ/mol	Joback Method
hvap	92.94	kJ/mol	Joback Method
log10ws	-9.51		Crippen Method
logp	7.447		Crippen Method
mcvol	349.880	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	2846.00		NIST Webbook
rinpol	2846.00		NIST Webbook
tb	984.82	K	Joback Method
tc	1205.90	K	Joback Method
tf	620.39	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.41	J/mol×K	984.82	Joback Method
cpg	1164.63	J/mol×K	1021.67	Joback Method
cpg	1178.67	J/mol×K	1058.51	Joback Method
cpg	1191.63	J/mol×K	1095.36	Joback Method
cpg	1203.58	J/mol×K	1132.21	Joback Method
cpg	1214.62	J/mol×K	1169.05	Joback Method
cpg	1224.84	J/mol×K	1205.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407613&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